A COMPLETE THEORETICAL ANALYSIS OF S-MATRIX ITS UNITARITY & IMPLICATIONS

By

SHUBHAM KUMAR

DU2019MSC0069

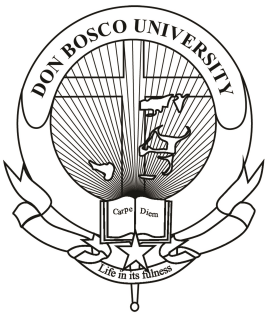
DEPARTMENT OF PHYSICS

A THESIS
SUBMITTED
IN PARTIAL FULFILLMENT OF THE REQUIREMENT
FOR THE DEGREE OF

MASTER OF SCIENCE

IN PHYSICS

To



ASSAM DON BOSCO UNIVERSITY

TAPESIA GARDENS, TAPESIA,
SONAPUR – 782 402
ASSAM – INDIA

JULY, 2021

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CERTIFICATE

This is to certify that this report titled

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is a bonafide record of the project work done by **Mr. SHUBHAM KUMAR** (Student ID DU2019MSC0069) at the Department of Physics, School of Fundamental & Applied Sciences, Assam Don Bosco University, under the guidance of **Dr. Debajyoti Dutta**, in partial fulfillment of the requirements of the *PSPR6012: Project Work* of the M.Sc. (Physics) curriculum.

Project Guide

Dr. Debajyoti Dutta

Place: ADBU, Tapesia

Date: July, 2021

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Place: ADBU, Tapesia

Date: July, 2021

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This is to certify that **SHUBHAM KUMAR** bearing **DU2019MSC0069** of **Department of Physics** has carried out the Project Work in a manner satisfactory to warrant its acceptance and also defended it successfully.

I wish him all success in future endeavours.

Examiners:

1. External Examiner

2. Internal Examiner

3. Internal Examiner

DECLARATION

I, SHUBHAM KUMAR, hereby declare that this report of the project work entitled "**A complete Theoretical Analysis of S-Matrix its Unitarity & implications**" is the record of the work carried out by me under the supervision of Dr. Debajyoti Dutta, Assam Don Bosco University. The content of this project did not form the basis for the award of any previous degree to me or to the best of my knowledge to anybody else. I also declare that the project has not been submitted by me for any research degree in any other university or institute.

This is being submitted to the Assam Don Bosco University for the degree of Master of Science in Physics.

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ABSTRACT

The S-Matrix is defined as an the limit of the Time evolution operator $\hat{U}(t_f,t_i)$ between asymptotic initial and final Hilbert/Fock spaces for a time-dependent scattering process, i.e. between $t\rightarrow\infty$ and $t\rightarrow$-∞. There unitarity encodes conservation of probabilities over time. The goal of this thesis is to do a thorough and complete analysis of this useful quantity in physics namely the S-Matrix, learn its construction specifically in the path integral formulation, and apply it in the forefront areas of Quantum gravity and String theory.The most trivial construction of S-Matrix can be done as an infinite perturbative series(Dyson Series) in the Canonical procedure of QFT.An analysis up to first order is done by introducing in -states and out-states and a Born approximated result is obtained. Further both the internal and external symmetries of the S-matrix are studied and their implications are drawn. An analytical proof of the unitarity of S-matrix is presented and further its implications are studied. A brief introduction to the Path integral formulations of QFT is done in order to construct the S-Matrix in the Path integral formulation, for this purpose various generating functionals are analysed. This is because greens functions are nothing but functional derivatives of the generating functionals also called partition functionals.Connected and amputated greens functionals and their generators are studied. As expected the S matrix in the Path integral formulation turned out to be a functional rather than a series or operator as in canonical QFT. After studying a general prescription to construct the S-matrix in Path integral formulation its unitarity is studied.This is very important if we want to construct any theory of quantum gravity then the S-matrix constructed for asymptotic interactions of the theory must be Unitary in order to preserve probability and respect causal conditions. At last introductory aspects of Quantum gravity and various approaches to quantize gravity is studied.The S-Matrix of Quantum gravity is also studied by Canonical Quantization of the Gauge Field.Introductory aspects String theory is studied via the Path integral formulation (Polyakov Integral) as it seems to be the natural language to construct a theory of Quantum gravity.Finally an attempt to construct S-matrix of these theories are done where the last sections are tributed to analyse the Unitarity of the S- matrix of the current string theory is done.As we know that the S-Matrix of these theories also needs to be consistent with the Unitarity criterion.However the Non Unitarity also seems to creep in some areas of standard model as well as 2D string theory,but that is beyond the scope of this work.Our sole aim is to provide a detailed analysis of the S-Matrix,the physics that comes with it,its uses, Unitarity and its implications.

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CHAPTER 1

INTRODUCTION

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1.1 Introduction

The main goal of this thesis is to do a complete analysis of one of the most important quantities in high energy physics i.e the **S-Matrix**.The analysis will be comprehensive ,thorough and self sufficient.We start with a formal introduction of the S-Matrix and discuss the major differences in two major formulations of modern Quantum field theory(QFT)namely, the Canonical formalism vs the Path integral formulation.Although the former i,e the Canonical formalism is used often by theorists as it seems most natural way to quantize a theory by invoking canonical commutation relation and seems sufficient.However we have learnt that although this approach is very powerful it seems to fail beyond the standard model, and is miserable enough when applied to construct theories of Quantum gravity.Path integral formalism on the other hand seems to be more powerful in approaching the modern problems in String theory and Quantum gravity.This is expected because the path integral formalism has its roots in one of the most fundamental laws of nature i,e the extremization of the action or the **action principle** itself. This is what has been noticed and applied by many giants,Feynman and Hawking to name a few.Path integral formulation can be easily generalised to the theory of Quantum gravity and String theory ,although the mathematics seems to be very tedious but the results seems promising.

Our study starts with the analysis of the S-matrix in the canonical QFT in chapter 2 where we study its properties ,symmetries,its uses and its general structure. We will try to visualise its action in the matrix form as well as in physical space, and we finally obtain its expression in Perturbative form and an Analytical expression of 1st order.At the end of the chapter we discuss one of most sought after properties that the S-Matrix of any theory must have i,e its **Unitarity** and study its implications in the canonical QFT and Scattering theory.

We introduce the machinery of **Path integrals** in chapter 3 where in first few sections we discuss the general aspects and workings of the Path integrals in the regime of NRQM(Non Reltivistic Quantum Mechanics ,Just to get and idea and make the basics clear and then we move to the Path integral formulation of **field theories**.In the field theory Path integrals we will study important tool namely the **Generating functionals** which will help us in the construction of the S matrix in the Path integral formalism. We will also study the generalised **n-point correlators** and path integral formulation of **n-point Green's Function**.

Having developed all the tools ,we now start constructing the S-Matrix in the path integral formalism of QFT in chapter 4. We will extensively used the tools developed in the previous chapters. We will also dedicate one subsection for analysing the Unitarity of the S-matrix in the Path integral formalism. This is important because unlike the Canonical formalism the S matrix here is a complex functional instead of an operator that we are used to in the canonical formalism. It is important to keep in mind that unlike in Canonical formalism where most of the objects we deal with are some kind of operators we don't have any concept of operators in the path integral formalism.Most of the dynamical variables are **functionals** in the Path integral formalism

Finally in the last chapter we will apply all that we have learnt in the previous chapters and study the Path integral formalism of the Quantum gravirty and the String theory. As already mentioned this will be done in the Path integral formalism because it seems to be the natural language. At last we will try to construct S-matrix in both Quantum gravity and String theory by drawing analogies from chapter 4. It is worth mentioning that the construction will be somewhat unrigorous and is just used to demonstrate the importance of the S- matrix. We will conclude the thesis by asking ourselves why is the Unitarity principle so important in physics and in particular what the Unitarity of the S matrix tells us about the theory, as we know the mordern String theory came

into existence by studying the S matrix theory in. 70's so something deeper must be going on.

1.2 Canonical Vs Path Integral formalism

Historically There have been two different approaches to any Quantum Field Theory in the past. The first was developed primarily by Paul M Dirac in order to deduce Quantum Electrodynamics in 1927. Canonical Quantization is the term given to this method "the procedure By advocating fields as operators and introducing quantization via canonical uncertainty relations, this formulation takes a more direct approach to QFT. This is done in order to maintain maximal symmetries in the theory. As one can see, the term "canonical" denotes that we operate along the lines of the Hamiltonian formulation, which means that we already have a Hamiltonian (H) and the system dynamics are generated using canonical Poisson brackets/commutators. Although more general commutation connections are introduced in quantizing the theory of fields, this aids in the preservation of not only exterior but also internal symmetries.

The second method is referred to as the "Path integral method " in which Rather than quantizing the canonical variables q and p, and hence the canonical relations, we quantify a more fundamental quantity of every dynamical system, namely the action [**S**] itself.We treat particles (QM) or fields (QFT) as if they were simultaneously travelling or evolving through all possible paths in this formulation. Despite the fact that the mathematics is more complicated, this formulation is more fundamental because it is based on the fundamental principles of dynamics itself.

In the Canonical Quantization formulation a quantity called the "Scattering Matrix"(S-Matrix) plays a very fundamental role. Although it does not introduce any new physics to the formulation, it does provide additional insights into scattering phenomena and compliments the computations done via the Feynman diagrams. The "Unitarity" of this S-Matrix provides the mathematical basis for the probability conservation in all of Quantum field theories.

However in the Path integral Formulation, on the other hand, one does not explicitly perform a comprehensive analysis of the S-Matrix.It's a bit of a grey area, especially when it comes to its Unitarity condition.However, in order to preserve probability

(which is a necessary criteria for any formulation/ any physical theory), the sum of probability over all paths/field configurations must equal unity.This can be accomplished by creating a correct S matrix and demonstrating the Unitarity condition for it.This will be the main area of focus of this thesis.

1.3 Scattering Matrix(S-Matrix)

The S-matrix is defined as an the limit of the Time evolution operator $\hat{U}(t_f,t_i)$ between asymptotic initial and final Hilbert spaces for a time-dependent scattering process, i.e. between $t\rightarrow\infty$ and $t\rightarrow\text{-}\infty$.There unitarity encodes conservation of probabilities over time.More formally, in the context of QFT, the S-matrix is defined as the unitary matrix connecting sets of asymptotically free particle states (the in-states and the out-states) in the Hilbert space of physical states. A multi-particle state is said to be free (non-interacting) if it transforms under Lorentz transformations as a tensor product, or direct product in physics. Asymptotically free then means that the state has this appearance in either the distant past or the distant future.

1.3.1 The Power of the S -Matrix

In particle accelerators, physicists measure the following quantities:

- cross sections of scattering processes
- masses of stable particles
- magnetic moments of elementary particles
- life of unstable particles

The task is to theoretically predict the measured values. To this end, physicists mainly use two concepts, namely,

- the S -matrix and
- n -point correlation functions/Greens Functions

Roughly speaking, the two concepts are equivalent. The S -matrix encodes the transition probabilities of scattering processes. In fact, the S -matrix knows all about elementary particles.

- The S -matrix enables us to compute the cross sections of scattering processes.
- The singularities of the S -matrix refer to the masses of stable particles.
- Analytic continuation of the S -matrix in momentum space tells us the masses of unstable particles (also called resonances) and their lifetimes.
- The S -matrix allows us to compute the full correlation functions by the magic Gell-Mann-Low formula. This way, for example, we get so-called form factors which yield the magnetic moments of elementary particles (e.g., the anomalous magnetic moment of the electron and the muon).

While the S-matrix may be constructed for any quantum mechanical scattering process, we're mainly interested in the asymptotically free particles scattering and interaction scenario. We'll address this using the field theory formulation, although a brief Introduction will be given in terms of the ordinary Quantum mechanics so as to draw analogies and provide the reader with a better insights and understanding of the underlying steps.We begin with a brief overview of the time evolution operator in conventional non relativistic quantum mechanics, then move on to the interaction picture, and ultimately to the time evolution operator for fields using the path integral method. Finally, we'll set the needed restrictions on a suitable S-Matrix and then establish its unitarity for any general situation. The goal of this study is to provide yet another evidence that the S matrix is unitary even when using the Path integral formulation. These are the reasons for this type of action. For starters, the unitarity condition is one of the most basic prerequisites for a theory to be considered physically acceptable. Second, it's preferable to have as unambiguous a proof scheme as feasible, with the process ensuring unitarity easily identified. Third, given the wide range of Lagrangians seen in modern quantum field theories one would like to know what criteria, to put on the regularisation procedure, etc., that may guarantee that the S matrix is unitary.

CHAPTER 2

S-Matrix analysis in Canonical QFT

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2.1 Time Evolution

In general, physical systems are dynamic, meaning they change over time. Newton's laws of motion explain the dynamics of classical mechanical systems, while Maxwell's equations determine the dynamics of the classical electromagnetic field. Although some unification is provided in terms of Hamilton's principle, a universal manner of articulating the laws of classical dynamics, either Newton's equations or Maxwell's equations constitute laws of physics whose form is specific to the kind of system being discussed. We need a way to explain the dynamical properties of quantum systems, i.e. given the state $\Psi(0)$ of a quantum system at some initial time t = 0, we need a physical rule that tells us what the state will be at some later time t, i.e. a quantum law of evolution. Given that a state vector is a repository for all known information about a system, we need a general physical law to explain how this information evolves over time in response to the physical circumstances in which the system of interest finds itself. It's to be expected that the details of this law will differ from system to system, but it turns out that the law of evolution may be described in a fashion that applies to all physical systems, similar to how Hamilton's principle allows for the concise expression of classical dynamical laws. Schrodinger's equation is, of course, the quantum law of evolution.Time evolution refers to the change in state caused by the passage of time in systems having internal states (also called stateful systems). Time does not have to be a continuous quantity in this formulation; it may be discrete or even finite. The laws of classical mechanics control the temporal development of a group of rigid bodies in classical physics. These principles, in their most basic form, describe the connection between forces acting on bodies and their acceleration as determined by Newton's equations of motion. Hamiltonian or Lagrangian mechanics may also be used to explain these concepts in a more abstract way.

Other stateful systems may benefit from the notion of temporal evolution. Stateful systems are often described in terms of both states and observable values. Time evolution may also refer to the change in observable quantities in such systems. This is especially important in quantum physics, where the Schrödinger and Heisenberg pictures of time evolution are (largely) identical.Time, unlike position, is not an observable quantity in quantum physics. There is no Hermitian operator with eigenvalues equal to the system's time, and time is just a parameter, not a measurable entity. So, according to the

relativity theory's teachings, time and position are not on a same footing. The equality is restored in relativistic quantum field theories by degrading the position down to the parameter level.In short we first have to understand the process of time evolution and for that it is necessary to introduce the mathematical formalism of the "Time evolution operator" $[\hat{U}(t_f,t_i)]$

2.2 Time Evolution operator

In Quantum Mechanics, we know that every system has many quantum states. As a passage of time new states are evolved. What we wish to do is to find a relation between these initial states and the evolved states. For this purpose we use a linear operator which evolves the states over time which is famously called the **Time Evolution Operator**. Let us see the various representations of this time evolution operator in different pictures and understand how it plays a fundamental role in ensuring the Unitarity of our final S Matrix.We start with the Schrödinger picture with a free non interacting Hamiltonian and subsequently move towards a more general representation in the Interaction Picture

2.2.1 Schrödinger Picture with free Non Interacting Hamiltonian

Let's start at the beginning and get the equation of motion for a system in general quantum state $\Psi(t)$ and its time evolution through the time propagator. We're looking for quantum motion equations that are analogous to Newton's — or, more precisely, Hamilton's — classical motion equations. How does this state vary with time if we know it at time $\Psi(t_i)$ How do we calculate $\Psi(t_f)$for a future time $t_f > t_i$?In this case, we'll rely on our intuition, which is primarily based on classical mechanics. We will not explicitly demonstrate the spatial dependency of the state in the following section to keep notation to a minimum.

A major postulate of Quantum mechanics also known as the famous Schrödinger equation states that for any system in a general quantum mechanical state evolves according

to the equation

$$\iota\hbar\frac{d\Psi(t)}{dt} = H\Psi(t) \tag{2.1}$$

The most general solution to the above equation is given as

$$|\Psi(t_{\mathrm{f}})\rangle = e^{-i(t_{\mathrm{f}}-t_{\mathrm{i}})\hat{H}/\hbar}|\Psi(t_{\mathrm{i}})\rangle \tag{2.2}$$

where the exponential term

$$e^{-iH(t_{\mathrm{f}}-t_{\mathrm{i}})} = \hat{U}(t_{\mathrm{f}}, t_{\mathrm{i}})$$

is known as the quantum mechanical **time evolution operator**.In general for a quantum particle travelling from a point (x_a, t_a) to another point (x_b, t_b) the matrix element U of the time evolution operator $\hat{\mathrm{U}}$ is given by

$$U(x_b, t_b; x_a, t_a) = \left\langle x_b \middle| \hat{U}(x_b, t_b; x_a, t_a) \middle| x_a \right\rangle = \left\langle x_b \middle| e^{-i(t_b-t_a)\hat{H/\hbar}} \middle| x_a \right\rangle \tag{2.3}$$

It is worth mentioning that We start by assuming causality: $|\Psi(t_i) >$ precedes and determines $|\Psi(t_f) >$, which is crucial for deriving a deterministic equation of motion. Also, as usual, we assume time is a continuous variable:

In case of Quantum field theory the matrix element of time evolution operator analogically known as the **Transition Operator** for a field (consider a scalar field Φ) evolving from an initial field configurationΦ_i to a final Configuration Φ_f is given by

$$\left\langle \Phi_f \middle| e^{-i(t_f-t_i)\hat{H}} \middle| \Phi_i \right\rangle \tag{2.4}$$

where $\hat{H} = \int d^3x.\mathcal{H}$ is the total Hamiltonian of the system and $\mathcal{H}$ is the Hamiltonian density.

2.2.2 Properties of time evolution operator/Transition operator(For time independent non interacting hamiltonians)

1. Unitarity: This is the most important criterion for any time evolution operator. It says that

$$\hat{U}\hat{U}^{\dagger} = 1 \tag{2.5}$$

This criterion is must for giving correct probabilistic interpretation to any wave functionΨ or any field Φ.The conservation of probability in quantum mechanics and QFT comes from this Unitarity condition.As we know that sum of all probabilities should be equal to unity.

2. Time ordering/Causality: Another important criterion for any time evolution operator is the "time order" that is the order in which it acts on the concerned state/ field.This is important in order to prevent any theory from breaking the "causality".Hence for any state/field Φ evolving from timet_1 to time t_n where the chronological order is from time

$$t_1 - - - - - - - - - - - - - - - - > t_k - - - - - - - - - - - - - - - - > t_n$$

The evolution operator $\hat{U}(t_n, t_1)$ between the states $\Phi(t_n)$ and $\Phi(t_1)$ must follow the semi group property given by

$$\hat{U}(t_n, t_1) = \hat{U}(t_n, t_k).\hat{U}(t_k, t_1) \tag{2.6}$$

Note that this property directy comes from the Hermitian nature of the Hamiltonian operator $\hat{H}$.

$$\hat{H} = \hat{H}^{\dagger}$$

This is guaranteed by the fact that the Hamiltonian is Independent of time.(Atleast in the above section.

2.2.3 Interaction Picture and Time evolution

Now we shift our attention to a more general case of time dependent hamiltonians, which indded is the case for many Interaction theories. Suppose that we have a Hamiltonian H, which we split into a free part H_o and an interacting part H_I, i.e.

$$H = H_o + H_I$$

We will work in the interaction picture here and assume units such that the reduced Planck constant $\hbar$ is 1.

In the interaction picture, the evolution operator U defined by the equation

$$\Psi(t) = U(t, t_0)\Psi(t_0) \tag{2.7}$$

is called the Dyson operator. We have

$$U(t, t) = I$$

$$U(t, t_0) = U(t, t_1)U(t_1, t_0)$$

$$U^{-1}(t, t_0) = U(t_0, t)$$

Now we differentiate the equation (2.7) both sides with respect to t and put the initial condition i.e

$$\frac{d\Psi(t)}{dt} = \frac{dU(t, t_0)}{dt}\Psi(t_0) + U(t, t_0)\frac{d\Psi(t_0)}{dt} \tag{2.8}$$

$$\frac{d\Psi(t)}{dt} = \frac{dU(t, t_0}{dt}\Psi(t_0) \tag{2.9}$$

In interaction picture

$$i\hbar\frac{d\Psi(t)}{dt} = H_I(t)\Psi(t), \qquad \hbar \to 1 \tag{2.10}$$

$$\frac{d\Psi(t)}{dt} = H_I(t)\Psi(t) = -iH_I(t)\Psi(t) \tag{2.11}$$

then the equation becomes

$$i\frac{dU(t, t_0)}{dt} = H_I(t)\Psi(t) \tag{2.12}$$

$$i\frac{dU(t,t_0)}{dt} = H_I(t)U(t,t_0)\Psi(t_0) \tag{2.13}$$

Equation 2.13 is commonly known as **Tomonaga–Schwinger equation** integrating the above equation from t_i to t_f

$$\int_{t_i}^{t_f} dU(t,t_0) = \int -iH_I(t)U(t,t_0)\,dt$$

$$U(t_f,t_0) - U(t_i,t_0) = -i\int H_I(t_1)U(t,t_0)\,dt_1 \tag{2.14}$$

put $t_i = t_0$ and $t_f = t$, since $U(t_0,t_0) = 1$

$$U(t_f,t_0) = U(t,t_0) = 1 - i\int H_I(t_1)U(t_1,t_0)\,dt_1 \tag{2.15}$$

which leads to Neumann series and the equation becomes

$$\begin{aligned} U(t,t_0) = 1 - i\int_{t_0}^{t} dt_1 H_I(t_1) + (-i)^2\int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2 H_I(t_1)H_I(t_2)... \\ + (-i)^n\int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2...\int_{t_0}^{t_{n-1}} dt_n H_I(t_1)H_I(t_2)...H_I(t_n) + ... \end{aligned} \tag{2.16}$$

since $t_1 > t_2 > ...t_n$, fields are time-ordered and it is convenient to introduce an operator $\mathcal{T}$ called "Time-ordering" operator which is given as

$$U(t,t_0) = (-i)^n\int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2...\int_{t_0}^{t_{n-1}} dt_n\mathcal{T}[H_I(t_1)H_I(t_2)...H_I(t_n)]$$

By making the integration simpler we can write it as

$$S_n = \int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2...\int_{t_0}^{t_{n-1}} dt_n K(t_1,t_2,...t_n)$$

Let us assume that K is symmetric in its arguments and define

$$I_n = \int_{t_0}^{t} dt_1\int_{t_0}^{t} dt_2...\int_{t_0}^{t} dt_n K(t_1,t_2,...t_n)$$

so we can say the region of integration can be broken into $n!$ sub-regions by $t_1 > t_2 > ... > t_n, t_2 > t_1 > ... > t_n$. The integral in each of these sub-regions is the same and

equal to S_n because of the symmetry of K, hence we can write ,

$$S_n = \frac{1}{n!} I_n$$

By using the above identity ,we can write the previous integral as

$$U_n = \frac{(-i)^n}{n!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 ... \int_{t_0}^{t} dt_n \mathcal{T} H_I(t_1) H_I(t_2) ... H_I(t_n) \tag{2.17}$$

summing up all the terms,therefore we get the Dyson's theorem for the Dyson series as

$$U(t, t_0) = \sum_{n=0}^{\infty} U_n(t, t_0) = \mathcal{T} e^{-i \int_{t_0}^{t} d\mathcal{T} H_I(\mathcal{T})} \tag{2.18}$$

2.3 S -Matrix and Scattering Theory in Canonical QFT

2.3.1 S-Matrix as the limit of Time evolution operator(Perturbative Expansion form)

The direct way to define the S-matrix start with consideration of Interaction picture. Let us consider the Hamiltonian H to be split into the part H_0 and the interaction $H_I, H = H_0 + H_I$. As we know the operators behave as free field operators in this picture and the state vectors have dynamics according to the interaction H_I.

Let $|\Psi(t)\rangle$ be a state that has evolved from a free initial state $|\Phi_i\rangle$. Then the S-matrix element is defined as the projection of this state on the final state $|\Phi_f\rangle$. Therefore,

$$S_{fi} \equiv \lim_{t\to+\infty} \langle\Phi_f|\Psi(t)\rangle \equiv \langle\Phi_f|S|\Phi_i\rangle \tag{2.19}$$

where S is the S-operator. The great advantage of this definition as that the time-evolution operator U evolving a state in the interaction picture.

$$U(t,t_0) = \mathcal{T}e^{-i\int_{t_0}^{t} d\mathcal{T}H_I(\mathcal{T})}$$

where $\mathcal{T}$ denotes the time-ordered product. Expressed in this operator,

$$S_{fi} = \lim_{t_2\to+\infty} \lim_{t_1\to-\infty} \langle\Phi_f|U(t_2,t_1)|\Phi_i\rangle \tag{2.20}$$

from which we can write $S = U(\infty,-\infty)$ expanding using the knowledge about U gives a Dyson series ,

$$S_n = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 ... \int_{-\infty}^{\infty} dt_n \mathcal{T}[H_I(t_1)...H_I(t_n)]$$

or ,in terms of Hamiltonian Density,

$$S = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dx_1^4 ... \int_{-\infty}^{\infty} dx_n^4 \mathcal{T}[\mathcal{H}_I(t_1)...\mathcal{H}_I(t_n)]$$

Being a special type of time-evolution operator, S is unitary. For any initial state and any final state one finds

$$s_{fi} = \langle \Phi_f | S | \Phi_i \rangle = \left\langle \Phi_f \middle| \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dx_1^4 ... \int_{-\infty}^{\infty} dx_n^4 \mathcal{T}[\mathcal{H}_I(t_1)...\mathcal{H}_I(t_n)] \middle| \Phi_i \right\rangle \quad (2.21)$$

2.3.2 The S Operator

From Eq 2.21 , we can find any given S_{fi} component of the S Matrix, such as the $f = 2$ final state,

$$\langle f = 2 \| F \rangle = \left\langle f = 2 \middle| \sum_f S_{fi} \middle| f \right\rangle = \langle f = 2 | \underbrace{(S_{1i}|f = 1\rangle + S_{2i}|f = 2\rangle + S_{3i}|f = 3\rangle + ..)}_{(S_{\text{oper }1i} + S_{\text{oper }2i} + ...)|i\rangle = S_{\text{oper }}|i\rangle}$$
$$= \langle f = 2 \, | S_{2i} | \, f = 2 \rangle + (\text{ many zero terms }) = S_{2i} = \langle f = 2 \, | S_{\text{oper}} \, | \, i \rangle \, .$$

Hence In general,

$$S_{fi} = \langle f \, | S_{\text{oper}} \, | \, i \rangle$$

This operator Sandwiched between the initial and final states is called the S-Operator

2.3.3 Expanding S_{oper}

S_{oper} can be expanded (in a Taylor series like $e^x = 1 + x + x^2/2! + x^3/3! + \ldots$) as

$$\begin{aligned} S_{\text{oper}}\ (t_f, t_i) &= e^{-i \int_{t_i}^{t_f} H_I^I(t) dt} = I - i \int_{t_i}^{t_f} H_I^I(t_1)\, dt_1 \\ &- \frac{1}{2!} T \left\{ \left(\int_{t_i}^{t_f} H_I^I(t_1)\, dt_1 \right) \left(\int_{t_i}^{t_f} H_I^I(t_2)\, dt_2 \right) \right\} + \ldots \\ &= \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{t_i}^{t_f} \ldots . \int_{t_i}^{t_f} T \left\{ H_I^I(t_1)\, H_I^I(t_2) \ldots H_I^I(t_n) \right\} dt_1 dt_2 \ldots dt_n \end{aligned} \quad (2.22)$$

If the H_I^I above were numeric functions of time, it wouldn't really matter what order, with respect to the t_n, we carry out the integrations in. However, since they are comprised of operators that act on a ket state to their right, , we have to be sure

that at each point in the integration, the time wise earliest operators are acting first. The operation of the operators must occur in the order they occur in nature, in time sequence. So, the earliest operator must operate on the ket first, i.e., it must be furthest to the right. The next earliest to operate must be second from the right, etc. This means that at each point in the n dimensional space where each axis is a different t_n, the H_I^I dependent on the earliest time of the t_n should act first, the H_I^1 dependent on the next earliest of the t_n should act next, etc. See Figure below for a two dimensional illustration of this, where we are integrating over the $t_1 - t_2$ plane.

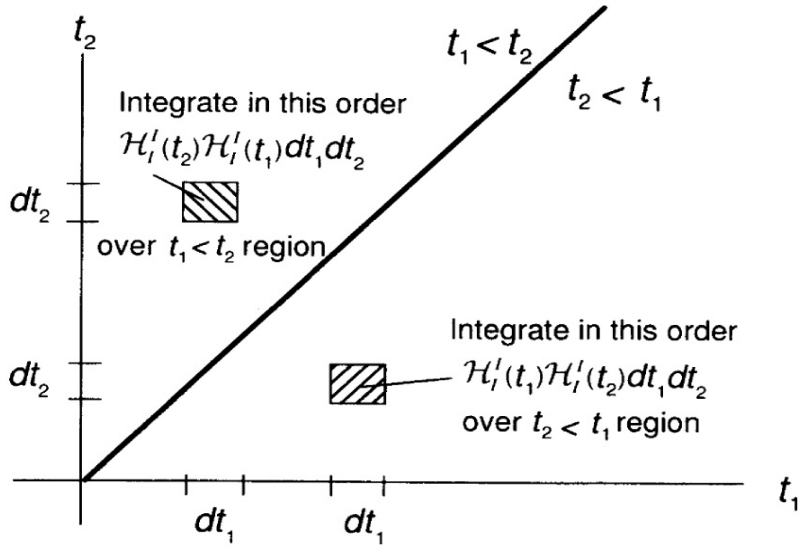


Figure 2.1: Time-ordering of integrand in t_n space

We indicate this ordering with the time ordering operator symbol $\mathcal{T}$ in the integrands . The order of the integrand operators is rearranged as we integrate over all t_n dimensions, such that the operators are time ordered at every point $(t_1, t_2, \ldots t_n)$

Taking our integration limits to infinity in both space and time, equation 2.23 is turned into the time ordered infinite spacetime S_{oper} , i.e., the Dyson expansion of the S operator,

$$S = S_{\substack{\text{oper} \\ V\to\infty}}\left(t_f \to \infty, t_i \to -\infty\right) = e^{-i\int_{-\infty}^{\infty}\mathcal{H}_I' d^4x}$$

Which on expansion gives

$$S=\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}.....\int_{-\infty}^{\infty}T\left\{\mathcal{H}_I^I\left(t_1\right)\mathcal{H}_I^I\left(t_2\right)\ldots\mathcal{H}_I^I\left(t_n\right)\right\}d^4x_1d^4x_2\ldots d^4x_n$$

SPECIAL NOTE: Above equation is the usual definition for the term "S operator" as used in QFT. Infinite time and space, along with time ordering, are assumed for the more general case of arbitrary time and space limits, in what we have been calling S_{oper} . So a big difference between S_{oper} and S is that time integration and volume of interaction for the latter are always infinite. From now on, when we use the term "S operator", unless otherwise stated.

2nd NOTE: Similarly, the S matrix elements S_{fi} in the literature usually correspond to the values for infinite time duration and infinite volume of the interaction. For us, they could represent either case, of finite time/volume or infinite time/volume, but from here on, unless otherwise specified, they will correspond to the infinite time/volume case.

$$S=\underbrace{I}_{S^{(0)}}\underbrace{-i\int_{-\infty}^{\infty}\mathcal{H}_l^I\left(x_1\right)d^4x_1}_{S^{(1)}}\underbrace{-\frac{1}{2!}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}T\left\{\mathcal{H}_I^l\left(x_1\right)\mathcal{H}_I'\left(x_2\right)\right\}d^4x_1d^4x_2}_{S^{(2)}}+.....=\sum_{n=0}^{\infty}S^{(n)}$$

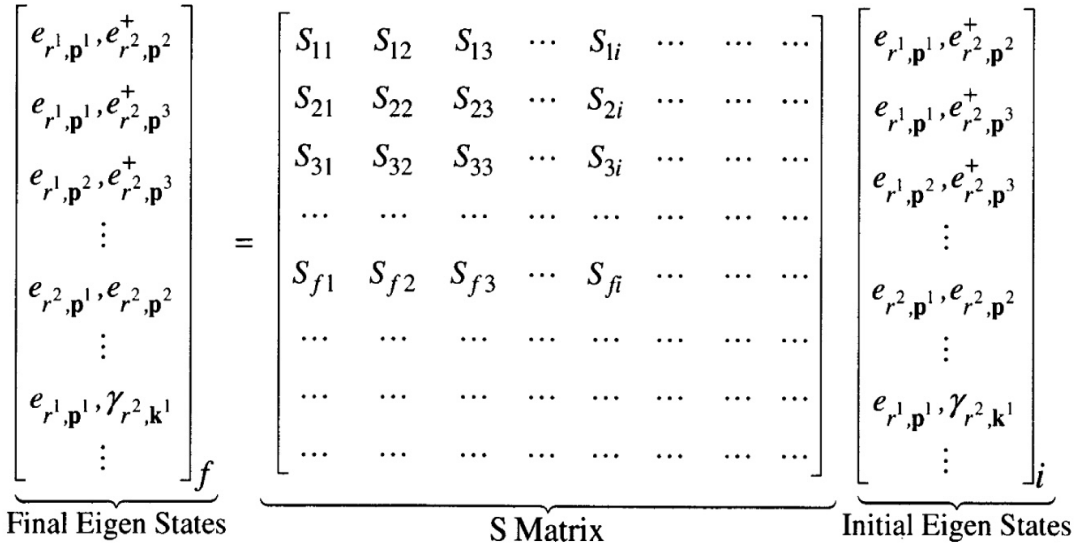
2.3.4 Ways to Visualize the S Operator

2.3.4.1 Matrix form

In a quantum scattering process different interactions have different probabilities to occur. So to keep track of each and every possible interaction, or to keep track of the individual probabilities for each to occur we use the machinery of **S-Matrix** shorthand for **Scattering Matrix** (since each of these interactions is considered a scattering process).

Consider a column vector for which each component represents a different initial (incoming) quantum eigenstate (typically multiparticle), as on the RH side of

each component of the column vector on the LH represents a different final (outgoing)



eigenstate.

The Probability of a certain transition occurring is equal to the square of the absolute value of each component of the S Matrix linking an initial and final state. For instance, the chance of the first initial state, consisting of an electron and positron with specific spins and momenta, interacting to form the second end state, consisting of an electron and positron with somewhat different specific spins and momenta, is

$S_{21}^{\dagger} S_{21} = |S_{21}|^2 =$ probability of 1st eigenstate transitioning to 2nd.

As a result, each component of the S Matrix, S_{fi}, represents a transition amplitude for a specific response (scattering event, transition, interaction) between particles in certain eigenstates, as defined in section 2.1. From here on out, our job is to figure out how to calculate S_{fi} for any given interaction.

Keep in mind that the S Matrix is huge, almost infinite, because it includes not only all possible types of interactions, but also all possible momenta magnitudes and directions for each type (all possible eigenstates), and many (most) of the components of the above matrix is equal zero, because many interactions such as $(e, \gamma \rightarrow e, e^{+})$ are impossible because charge is not conserved.The probability that the particles in the 3^{rd} (usually multiparticle) final eigenstate will be measured to be unchanged from the initial ones is represented by $|S_{33}|^2$.

2.3.4.2 Physical Space Visualisation

Lets visualise physically what is happening for this ,Consider an example of an initial e^- and e^+ annihilating one another to become a virtual photon, which in turn mutates into a final μ^- and μ^+. Each possible outgoing state could have different momenta for the two particles (with same total momentum). Each such state would be a different possible (multiparticle) final eigenstate. Each would, in general, have a different probability of being measured from the other final eigenstates. Of course, we could also have final states of fermion pairs e^-e^+ or $\tau^-\tau^+$, each with many different possible momenta states. So,

$$\overbrace{\left|e^-_{r^1\mathbf{p}^1}, e^+_{r^2\mathbf{p}^2}\right\rangle}^{|i=1\rangle} \Rightarrow S_{oper} \Rightarrow \underbrace{S_{11}\overbrace{\left|e^-_{r^1\mathbf{p}^1}, e^+_{r^2\mathbf{p}^2}\right\rangle}^{|f=1\rangle} + S_{21}\overbrace{\left|e^-_{r^1,\mathbf{p}^3}, e^+_{r^2,\mathbf{p}^4}\right\rangle}^{|f=2\rangle} + \ldots}_{\text{electron-positron final states}} + \underbrace{S_{\mu 1 1}\left|\mu^-_{r^1,\mathbf{p}^1}, \mu^+_{r^2,\mathbf{p}^2}\right\rangle}_{\text{muon-antimuon final state}} + \ldots$$

Hence S_{oper} converts the initial eigenstate into a final general state sum of eigenstates where the square of the absolute magnitude of the coefficient of each final eigenstate, S_{fi}, equals the probability of measuring that final eigenstate.

2.3.4.3 Visualisation in Fock Space

In Fock space every eigenstate can be visualized as a separate axis in an infinite (abstract) dimensional space, the S_{oper} can be visualized as a sort of abstract "rotation" in that space. The initial state vector $|i\rangle$ is "rotated" by the S_{oper} into a new vector with components along the eigenstate basis axes. In Fig. 2-2, we illustrate this for a final general state composed of only two component eigenstates.

This should seem reasonable, as S_{oper} has the form of a function $e^{-i\theta}$ where θ is the angle a complex quantity (a phasor) in complex space is rotated through. Also, , we see that the norm (abstract "length" $= 1$) of the state vector is unchanged under the operation S_{oper} , i.e., we have a different final vector but it has the same magnitude. This is what happens in rotation.

By close analogy, a complex number can be represent as $z = Re^{i\phi}$ with length R.

Operating on z with $e^{-i\theta}$ is $e^{-i\theta}z = e^{-i\theta}Re^{i\phi} = Re^{-i\theta+i\phi}$, which has the same length R, but is rotated through θ.

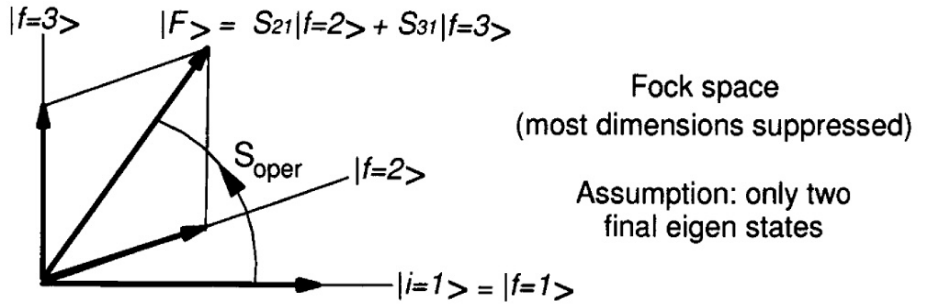


Figure 2.2: The action of the S operator Visualised in Fock space

2.3.5 What is H_I in the I.P. of QFT?

We've seen that all of the elements in the perturbative expansion of the S-Matrix include time ordered expressions for the interaction Hamiltonian H_I. The interaction Hamiltonian H_I is different for various interaction types, i.e., different kinds of forces. Electromagnetic interactions are one thing, weak interactions are another, and strong interactions are yet a third. Our current aim is to find it in the most basic instances so that we may utilise this characteristics of the interacting hamiltonian to establish the unitarity of the S-Matrix later in this chapter's second last part. Recall that there is a general rule that the interaction Lagrangian (or wave equation, or Hamiltonian) for states in the S.P. of Relativistic QM is the same as that for fields in the I.P. of QFT. For free fields, the H.P. and I.P. are the same, so this is consistent with our prior work. Using this rule for quantum electrodynamics or QED) for an example , we can find the e/m interaction Hamiltonian $QED^{H_I^I}$ via

$$\mathcal{H}_I = -\mathcal{L}_I = -e\bar{\psi}(x)\gamma^\mu A_\mu(x)\psi(x) \quad QED^{H_I} = \int_V \mathcal{H}_I d^3x$$

and for QED, this can be used in the perturbative expansion of the S-Matrix(Dyson Series). In the I.P., fields (operators) behave like free fields, as we have seen. Given this, we take the fields $\psi, \bar{\psi}$, and A^μ as free fields (even though they are part of the interaction Hamiltonian). We leave further exploration for proving the unitarity of the perturbation form in the second last section of this chapter.

We will find that, similar to 3D volume, considering the integration time for the operation of S_{oper} to be very large, effectively infinite, will be advantageous in developing the mathematics of QFT. Fortunately, again as we will eventually see, the results using this assumption can be used to accurately predict real world experimental outcomes.

2.3.6 In States and Out States

There are several interactions that may occur in particle theory. A large number of different incoming particles can interact with one other. There are numerous final (and frequently distinct) sets of departing particles for each set of entering particles.

A state made up of multiple non-interacting particles can be thought of as a direct product of one-particle states under the inhomogeneaus Lorentz group. We use their four-momenta p^μ, spin z-component (or, for massless particles, helicity) σ, and, because we may now be dealing with more than one species of particle, an additional discrete label n : for the particle type, which includes a specification of its mass, spin, charge, and so on, to label the one-particle states. The general rule of transformation is:

$$\begin{aligned} U(\Lambda,a)\Psi_{p_1,\sigma_1,n_1;p_2,\sigma_2,n_2;\cdots} &= e^{\left(-ia_\mu\left(p_1^\mu+p_2^\mu+\cdots\right)\right)} \\ &\times\sqrt{\frac{\left(\Lambda p_1\right)^0\left(\Lambda p_2\right)^{0\cdots}}{p_1^0p_2^0\cdots}}\sum_{\sigma_1'\sigma_2'\cdots}D^{(j_1)}_{\sigma_1'\sigma_1}\left(W\left(\Lambda,p_1\right)\right)D^{(j_2)}_{\sigma_2'\sigma_2}\left(W\left(\Lambda,p_2\right)\right)\cdots \\ &\times\Psi_{\Lambda p_1,\sigma_1',n_1;\Lambda p_2,\sigma_2',n_2;\cdots} \end{aligned} \tag{2.23}$$

where $W(\Lambda,p)$ is the Wigner rotation , and $D^{(j_i)}_{\sigma'\sigma}(W)$ are the conventional $(2j+1)$-dimensional unitary matrices representing the three dimensional rotation group. (This is for massive particles; for any mass- less particle, the matrix $D^{(j)}_{\sigma'\sigma}(W(\Lambda,p))$ is replaced with $\delta_{\sigma'\sigma}\exp(i\sigma\theta(\Lambda,p))$ where θ is the infinitesimal transformation group parameter. The states are normalized as

$$\begin{aligned} &\left(\Psi_{p_1',\sigma_1',n_1',p_2',\sigma_2',n_2',\cdots},\Psi_{p_1,\sigma_1,n_1;p_2,\sigma_2,n_2;\cdots}\right) \\ &=\delta^3\left(\boldsymbol{p}_1'-\mathbf{p}_1\right)\delta_{\sigma_1'\sigma_1}\delta_{n_1'n_1}\delta^3\left(\mathbf{p}_2'-\mathbf{p}_2\right)\delta_{\sigma_2'\sigma_2}\delta_{n_2'n_2}\cdots \pm \text{ permutations} \end{aligned} \tag{2.24}$$

with the term ' $\pm$ permutations' included to take account of the possibility that it is

some permutation of the particle types $n'_1, n'_2, \cdots$ that are of the same species of the particle types $n_1, n_2, \cdots$ (its sign is -1 if this permutation includes an odd permutation of half-integer spin particles, and otherwise $+1$. .)

We often use an abbreviated notation, letting one Greek letter, say α, stand for the whole collection $p_1, \sigma_1, n_1; p_2, \sigma_2, n_2; \cdots$ In this notation, the previous equation is written simply as

$$(\Psi_{\alpha'}, \Psi_\alpha) = \delta(\alpha' - \alpha) \tag{2.25}$$

with $\delta(\alpha' - \alpha)$ standing for the sum of products of delta functions and Kronecker deltas appearing on the right-hand side of Eq. (2.24). Also, in summing over states, we write

$$\int d\alpha \cdots \equiv \sum_{n_1 \sigma_1 n_2 \sigma_2 \cdots} \int d^3 p_1 d^3 p_2 \cdots$$

In particular, the completeness relation for states normalized as in Eq. (2.25) reads

$$\Psi = \int d\alpha \Psi_\alpha (\Psi_\alpha, \Psi)$$

The transformation rule (2.23) is only possible for particles that for one reason or another are not interacting. Setting $\Lambda^\mu_{\ v} = \delta^\mu_{\ v}$ and $a^\mu = (0, 0, 0, \tau)$, for which $U(\Lambda, a) = \exp(iH\tau)$, Eq. (2.23) requires among other things that Ψ_α be an energy eigenstate

$$H\Psi_\alpha = E_\alpha \Psi_\alpha$$

with an energy equal to the sum of the one-particle energies

$$E_\alpha = p_1^0 + p_2^0 + \cdots$$

and with no interaction terms, terms that would involve more than one particle at a time.

On the other hand, the transformation rule (2.23) does apply in scattering processes at times $t \to \pm\infty$. As explained in the introduction in the typical scattering experiment we start with particles at time $t \to -\infty$ so far apart that they are not yet interacting, and end with particles at $t \to +\infty$ so far apart that they have ceased interacting. We therefore have not one but two sets of states that transform as in Eq. (2.23): **the 'in'**

and 'out' states ${\Psi_\alpha}^+$ and ${\Psi_\alpha}^-$ will be found to contain the particles described by the label α if observations are made at $t \to -\infty$ or $t \to +\infty$, respectively.

Note how this definition is framed. To maintain manifest Lorentz invariance, in the formalism we are using here, state-vectors do not change with time - a state-vector Ψ describes the whole spacetime history of a system of particles. (This is known as the Heisenberg picture, in distinction with the Schrödinger picture, where the operators are constant and the states change with time.) Thus we do not say that ${\Psi_\alpha}^\pm$ are the limits at $t \to \pm$ of a time-dependent state-vector $\Psi(t)$.

However, implicit in the definition of the states is a choice of the inertial frame from which the observer views the system; different observers see equivalent state-vectors, but not the same state-vector. In particular, suppose that a standard observer θ sets his or her clock so that $t = 0$ is at some time during the collision process, while some other observer $\mathcal{O}'$ at rest with respect to the first uses a clock set so that $t' = 0$ is at a time $t = \tau$; that is, the two observers' time coordinates are related by $t' = t - t$. Then if $\mathcal{O}$ sees the system to be in a state $\Psi, \mathcal{O}'$ will see the system in a state $U(1, -\tau)\Psi = \exp(-iH\tau)\Psi$. Thus the appearance of the state long before or long after the collision (in whatever basis is used by $\mathcal{O}$) is found by applying a time-translation operator $\exp(-iH\tau)$ with $\tau \to -\infty$ or $\tau \to +\infty$, respectively. Of course, if the state is really an energy eigenstate, then it cannot be localized in time - the operator $\exp(-iH\tau)$ yields an inconsequential phase factor $\exp(-iE_\alpha\tau)$. Therefore, we must consider wave-packets, superpositions $\int d\alpha g(\alpha)\Psi_\alpha$ of states, with an amplitude $g(\alpha)$ that is non-zero and smoothly varying over some finite range $\triangle E$ of energies. The 'in' and 'out' states are defined so that the superposition

$$\exp(-iH\tau)\int d\alpha.g(\alpha)\Psi_\alpha^\pm = \int d\alpha e^{-iE_x\tau}g(\alpha)\Psi_\alpha\pm$$

has the appearance of a corresponding superposition of free-particle states for $\tau \ll -1/\Delta E$ or $\tau \gg +1/\triangle E$, respectively

To make this concrete, suppose we can divide the time-translation generator H into two terms, a free-particle Hamiltonian H_0 and an interaction V

$$H = H_0 + V$$

in such a way that H_0 has eigenstates Φ_α that have the same appearance as the eigenstates Ψ_α^+ and Ψ_α^- of the complete Hamiltonian

$$H_0\Phi_\alpha = E_\alpha\Phi_\alpha$$
$$(\Phi_{\alpha'}, \Phi_\alpha) = \delta(\alpha' - \alpha)$$

Note that H_0 is assumed here to have the same spectrum as the full Hamiltonian H. This requires that the masses appearing in H_0 be the physical masses that are actually measured, which are not necessarily the same as the 'bare' mass terms appearing in H; the difference if there is any must be included in the interaction V not H_0. Also, any relevant bound states in the spectrum of H should be introduced into H_0 as if they were elementary particles."

The 'in' and 'out' states can now be defined as eigenstates of H, not H_0,

$$H\Psi_\alpha^\pm = E_\alpha\Psi_\alpha^\pm$$

Where Ψ_α^- is the In state and Ψ_α^+ represent the Out State. They satisfy the condition

$$\int d\alpha . e^{-iE_\alpha\tau} g(\alpha)\Psi_\alpha^\pm \to \int dx e^{-iE_\alpha\tau} g(\alpha)\Phi_\alpha \tag{2.26}$$

for $\tau \to -\infty$ or $\tau \to +\infty$, respectively. Eq.(2.26) can be rewritten as the requirement that:

$$\exp(-iH\tau)\int d\alpha g(\alpha)\Psi_\alpha^\pm \to \exp(-iH_0\tau)\int dx g(\alpha)\Phi_\alpha$$

for $\tau \to -\infty$ or $\tau \to +\infty$, respectively. This is sometimes rewritten as a formula for the 'in' and 'out' states:

$$\Psi_\alpha^\pm = \Omega(\mp\infty)\Phi_\alpha, \tag{2.27}$$

where

$$\Omega(\tau) \equiv \exp(+iH\tau)\exp(-iH_0\tau)$$

However, it should be kept in mind that $\Omega(\mp\infty)$ in Eq. (2.27) gives meaningful results only when acting on a smooth superposition of energy eigenstates.

One immediate consequence of the definition (2.26) is that the 'in' and 'out' states are normalized just like the free-particle states. To see this, note that since the left-

hand side of Eq. (2.26) is obtained by letting the unitary operator exp $(-iH\tau)$ act on a time-independent state, its norm is independent of time, and therefore equals the norm of its limit for $\tau \to \infty$, i.e., the norm of the right-hand side of Eq. (2.26):

$$\begin{aligned}&\int d\alpha.d\beta \exp\left(-i\left(E_\alpha - E_\beta\right)\tau\right) g(\alpha)g^*(\beta)\left(\Psi_\beta^\pm, \Psi_\alpha^\pm\right)\\ &= \int d\alpha.d\beta \exp\left(-i\left(E_\alpha - E_\beta\right)\tau\right) g(\alpha)g^*(\beta)\left(\Phi_\beta, \Phi_\alpha\right)\end{aligned}$$

Since this is supposed to be true for all smooth functions $g(\alpha)$, the scalar products must be equal

$$\left(\Psi_\beta^\pm, \Psi_\alpha^\pm\right) = \left(\Phi_\beta, \Phi_{\alpha.}\right) = \delta(\beta - \alpha)$$

It is useful for some purposes to have an explicit though formal solution of the energy eigenvalue equation

$$H\Psi_\alpha^\pm = E_\alpha \Psi_\alpha^\pm$$

satisfying the conditions (2.26). For this purpose, write the above equation as

$$\left(E_\alpha - H_0\right){\Psi_\alpha}^\pm = V{\Psi_\alpha}^\pm$$

The operator $E_\alpha - H_0$ is not invertible; it annihilates not only the freeparticle state Φ_α, but also the continuum of other free-particle states Φ_β of the same energy. Since the 'in' and 'out' states become just Φ_α for $V \to 0$, we tentatively write the formal solutions as Φ_x plus a term proportional to V :

$${\Psi_\alpha}^\pm = \Phi_\alpha + \left(E_x - H_0 \pm i\epsilon\right)^{-1} V\Psi_\alpha^\pm$$

or, expanding in a complete set of free-particle states,

$$\begin{aligned}\Psi_\alpha^\pm &= \Phi_\alpha + \int d\beta \frac{T_{\beta\alpha}^\pm \Phi_\beta}{E_\alpha - E_\beta \pm i\epsilon}\\ {T_{\beta\alpha}}^\pm &\equiv \left(\Phi_\beta, V\Psi_\alpha^\pm\right)\end{aligned} \tag{2.28}$$

with ϵ a positive infinitesimal quantity, inserted to give meaning to the reciprocal of $E_\alpha - H_0$. These are known as the **Lippmann-Schwinger Equation**, which is in Scattering theory equivalent to the Schrodiner equation.

It can be shown that Eq. (2.28), with a $+i\epsilon$ or $-i\epsilon$ in the denominator, satisfies the condition

$$\int d\alpha . e^{-iE_\alpha \tau} g(\alpha) \Psi_\alpha^\pm \to \int dx e^{-iE_\alpha \tau} g(\alpha) \Phi_\alpha$$

for $\tau \to -\infty$ or $\tau \to +\infty$, respectively for an 'in' or an 'out' state, respectively. For this purpose, consider the superpositions

$$\Psi_g^\pm(t) = \int d\alpha e^{-iE_n t} g(\alpha) \Psi_\alpha^\pm \tag{2.29}$$

$$\Phi_g(t) \equiv \int d\alpha e^{-iE_x t} g(\alpha) \Phi_\alpha$$

We want to show that ${\Psi_g}^+(t)$ and ${\Psi_g}^-(t)$ approach $\Phi_g(t)$ for $t \to -\infty$ and $t \to +\infty$, respectively. Using Eq. (2.28) in Eq. (2.29) gives

$$\Psi_{\mathrm{g}}^\pm(t) = \Phi_g(t) + \int d\alpha \int d\beta \frac{e^{-iE_\alpha t} g(\alpha) T_{\beta\alpha} \pm \Phi_\beta}{E_\alpha - E_\beta \pm i\epsilon}$$

Let us recklessly interchange the order of integration, and consider first the integrals

$$\mathscr{I}_\beta \pm \equiv \int d\alpha \frac{e^{-iE_a t} g(\alpha) T_{\beta x} \pm}{E_x - E_\beta \pm i\epsilon}$$

For $t \to -\infty$, we can close the contour of integration for the energy variable E_α in the upper half-plane with a large semi-circle, with the contribution from this semi-circle killed by the factor $\exp(-iE_\alpha t)$, which is exponentially small for $t \to -\infty$ and $\operatorname{Im} E_x > 0$. The integral is then given by a sum over the singularities of the integral in the upper halfplane. The functions $g(\alpha)$ and $T_{\beta\alpha}\pm$ may, in general, be expected to have some singularities at values of E_α with finite positive imaginary parts, but just as for the large semi-circle, their contribution is exponentially damped for $t \to -\infty$. (Specifically, $-t$ must be much greater than both the time-uncertainty in the wave-packet $g(\alpha)$ and the duration of the collision, which respectively govern the location of the singularities of $g(\alpha)$ and $T_{\beta x}\pm$ in the complex E_α plane.) This leaves the singularity in $(E_\alpha - E_\beta \pm i\epsilon)^{-1}$, which is in the upper half-plane for $\mathscr{I}_\beta -$ but not $\mathscr{I}_\beta +$ We conclude then that $\mathscr{I}_\beta^+$ vanishes for $t \to -\infty$. In the same way, for $t \to +\infty$ we must close the contour of integration in the lower half-plane, and so $\mathscr{I}_\beta{}^-$ vanishes in this limit. We conclude that $\Psi_{\mathrm{g}}^\pm(t)$ approaches $\Phi_g(t)$ for $t \to \mp\infty$, in agreement with the defining

condition

$$\int d\alpha . e^{-iE_\alpha \tau} g(\alpha) \Psi_\alpha^{\pm} \rightarrow \int dx e^{-iE_\alpha \tau} g(\alpha) \Phi_\alpha$$

2.3.7 S-Matrix defination from In-Out States

An experimentalist generally prepares a state to have a definite particle content at $t \rightarrow -\infty$, and then measures what this state looks like at $t \rightarrow +\infty$. If the state is prepared to have a particle content α for $t \rightarrow -\infty$, then it is the 'in' state Ψ_α^+, and if it is found to have the particle content β at $t \rightarrow +\infty$, then it is the 'out' state $\Psi_\beta -$. The probability amplitude for the transition $\alpha \rightarrow \beta$ is thus the scalar product

$$S_{\beta\alpha} = \left(\Psi_\beta^-, \Psi_\alpha^+\right) \tag{2.30}$$

This array of complex amplitudes is known as the S -matrix. If there were no interactions then 'in' and 'out' states would be the same, and then $S_{\beta\alpha}$ would be just $\delta(\alpha - \beta)$. The rate for a reaction $\alpha \rightarrow \beta$ is thus proportional to $|S_{\beta\alpha} - \delta(\alpha - \beta)|^2$. We shall see in detail in subsection 2.3.10 what $S_{\beta\alpha}$ has to do with measured rates and cross-sections.

Perhaps it should be stressed that 'in' and 'out' states do not inhabit two different Hilbert spaces. They differ only in how they are labelled: by their appearance either at $t \rightarrow -\infty$ or $t \rightarrow +\infty$. Any "in' state can be expanded as a sum of 'out' states, with expansion coefficients given by the S -matrix (2.30). Since $S_{\beta\alpha}$ is the matrix connecting two sets of orthonormal states, it must be unitary. We ll Prove its Unitarity in the last section and also discuss some of its implications.

2.3.8 Analytical form of S -Matrix(Born Approximation)

It is often convenient instead of dealing with the S -matrix to work with an operator S, defined to have matrix elements between free-particle states equal to the corresponding elements of the S -matrix:

$$(\Phi_\beta, S\Phi_\alpha) \equiv S_{\beta\alpha}$$

Recall the explicit though highly formal expression for the 'in' and 'out' states i.e

$$\Psi_\alpha^{\pm} = \Omega(\mp\infty)\Phi_\alpha,$$

yields a formula for the S -operator as :

$$S = \Omega(\infty)^{\dagger}\Omega(-\infty) = U(+\infty, -\infty)$$

where

$$U(\tau, \tau_0) \equiv \Omega(\tau)^{\dagger}\Omega(\tau_0) = \exp(iH_0\tau)\exp(-iH(\tau - \tau_0))\exp(-iH_0\tau_0)$$

This will be used in the next section to examine the Lorentz invariance of the S -matrix, a The methods of the previous section can be used to derive a useful alternative formula for the S -matrix. Let's return to Equation

$$\Psi_{\mathrm{g}}^{\pm}(t) = \Phi_g(t) + \int d\alpha \int d\beta \frac{e^{-iE_\alpha t} g(\alpha) T_{\beta\alpha} \pm \Phi_\beta}{E_\alpha - E_\beta \pm i\epsilon}$$

for the 'in' state Ψ^+, but this time take $t \to +\infty$. We must now close the contour of integration for E_α in the lower hatf- E_α -plane, and although as before the singularities in ${T_{\beta x}}^+$ and $g(\alpha)$ make no contribution for $t \to +\infty$, we now do pick up a contribution from the singular factor $(E_\alpha - E_\beta + i\epsilon)^{-1}$. The contour runs from $E_x = -\infty$ to $E_x = +\infty$, and then back to $E_\alpha = -\infty$ on a large semi-circle in the lower half-plane, so it circles the singularity in a clockwise direction. By the method of residues, this contribution to the integral over E_α is given by the value of the integrand at $E_\alpha = E_\beta - i\varepsilon$, times a factor $-2i\pi$. That is, in the limit $\epsilon \to 0+$, for $t \to +\infty$ the integral over α in equation has the asymptotic behavior

$${\mathscr{I}_\beta}^+ \to -2i\pi e^{-iE_\beta t} \int dx \delta(E_\alpha - E_\beta) g(\alpha) {T_{\beta\alpha}}^+$$

and hence, for $t \to +\infty$,

$$\Psi_g^+(t) \to \int d\beta e^{-iE_\beta t} \mathbf{\Phi}_\beta \left[g(\beta) - 2i\pi \int d\alpha \delta(E_x - E_\beta) g(\alpha) {T_{\beta\alpha}}^+ \right]$$

But expanding the superposition

$$\Psi_g^{\pm}(t) = \int d\alpha e^{-iE_n t} g(\alpha) \Psi_\alpha^{\pm}$$

for ${\Psi_g}^+$ in a complete set of 'out' states gives

$$ {\Psi_g}^+(t) = \int dx e^{-iE_\alpha t} g(\alpha) \int d\beta \Psi_\beta^- S_{\beta\alpha} $$

Since $S_{\beta\alpha}$ contains a factor $\delta\left(E_\beta - E_\alpha\right)$, this may be rewritten

$$ \Psi_g^+(t) = \int d\beta \Psi_\beta^- e^{-iE_\beta t} \int d\alpha g(\alpha) S_{\beta\alpha} $$

and, using the defining property (2.26) for 'out' states, this has the asymptotic behavior for $t \to +\infty$

$$ \Psi_g^+(t) \to \int d\beta \Phi_\beta e^{-iE_\beta t} \int d\alpha g(\alpha) S_{\beta\alpha} $$

Comparing this with our previous result, we find

$$ \int d\alpha g(\alpha) S_{\beta\alpha} = g(\beta) - 2i\pi \int dx \delta\left(E_\alpha - E_\beta\right) g(x) T_{\beta\alpha}^+ $$

or in other words

$$ S_{\beta\alpha} = \delta(\beta - \alpha) - 2i\pi\delta\left(E_\alpha - E_\beta\right) {T_{\beta\alpha}}^+ $$

This suggests a simple approximation for the S -matrix: for a weak interaction V, we can neglect the difference between 'in' and free-particle states in the expression ${T_{\beta\alpha}}^\pm \equiv (\Phi_\beta, V\Psi_\alpha^\pm)$ in which case $S_{\beta\alpha}$ becomes

$$ S_{\beta\alpha} \simeq \delta(\beta - \alpha) - 2i\pi\delta\left(E_\alpha - E_\beta\right)(\Phi_\beta, V\Phi_\alpha) $$

This is called **Born Approximation**.Which is reasonably good for very weak interactions.For higher order terms we had to turn to the Perturbative expression of the S-Matrix.

2.3.9 Symmetries of S-Matrix

In this section we will consider both what is meant by the invariance of the S-matrix under various symmetries, and what are the conditions on the Hamiltonian that will ensure such invariance properties .

2.3.9.1 Lorentz Invariance

For any proper orthochronous Lorentz transformation $x \to \Lambda x + a$, we may define a unitary operator $U(\Lambda, a)$ by specifying that it acts as follows

$$\begin{aligned} U(\Lambda,a)\Psi_{p_1,\sigma_1,n_1;p_2,\sigma_2,n_2;\cdots} &= \exp\left(-ia_\mu\left(p_1^\mu + p_2^\mu + \cdots\right)\right) \\ &\times \sqrt{\frac{\left(\Lambda p_1\right)^0\left(\Lambda p_2\right)^{0\cdots}}{p_1^0 p_2^0\cdots}} \sum_{\sigma_1'\sigma_2'\cdots} D^{(j_1)}_{\sigma_1'\sigma_1}\left(W\left(\Lambda,p_1\right)\right) D^{(j_2)}_{\sigma_2'\sigma_2}\left(W\left(\Lambda,p_2\right)\right)\cdots \\ &\times \Psi_{\Lambda p_1,\sigma_1',n_1;\Lambda p_2,\sigma_2',n_2;\cdots} \end{aligned}$$

on either the 'in' or the 'out' states. When we say that a theory is Lorentz-invariant, we mean that the same operator $U(\Lambda, a)$ acts as above on both 'in' and 'out' states. Since the operator $U(\Lambda, a)$ is unitary, we may write

$$S_{\beta\alpha} = \left(\Psi_\beta^-, \Psi_\alpha^+\right) = \left(U(\Lambda,a)\Psi_\beta - U(\Lambda,a)\Psi_\alpha^+\right)$$

so using (2.23), we obtain the Lorentz invariance (actually, covariance) property of the S -matrix: for arbitrary Lorentz transformations $\Lambda^\mu{}_v$ and translations a^μ,as

$$\begin{aligned} &S_{p_1',\sigma_1',n_1';p_2',\sigma_2',n_2',\cdots,,p_1,\sigma_1,n_i;p_2,\sigma_2,n_2;\cdots} \\ &= \exp\left(ia_\mu\left(p_1^\mu + p_2^\mu + \cdots - p_1'^\mu - p_2'^\mu - \cdots\right)\right) \\ &\times \sqrt{\frac{\left(\Lambda p_1\right)^0\left(\Lambda p_2\right)^0\cdots\left(\Lambda p_1'\right)^0\left(\Lambda p_2'\right)^0\cdots}{p_1^0 p_2^0\cdots p_1'^0 p_2'^0\cdots}} \\ &\times \sum_{\bar\sigma_1\bar\sigma_2\cdots} D^{(j_1)}_{\bar\sigma_1\sigma_1}(W(\Lambda,p_1)) D^{(j_2)}_{\bar\sigma_2\sigma_2}\left(W\left(\Lambda,p_2\right)\right)\cdots \\ &\times \sum_{\bar\sigma_1'\bar\sigma_2'\cdots} D^{\left(j_1'\right)}_{\bar\sigma_1'\sigma_1'}\left(W^*\left(\Lambda,p_1'\right)\right) D^{\left(j_2'\right)}_{\bar\sigma_2'\sigma_2'}\left(W^*\left(\Lambda,p_2'\right)\right)\cdots \\ &\times S_{\Lambda P_1',\bar\sigma_1',n_1';\Lambda p_2',\bar\sigma_2^t,n_2',\cdots,\Lambda p_1,\bar\sigma_1,n_1;\Lambda\rho_2,\bar\sigma_2,n_2;\cdots} \end{aligned}$$

(Primes are used to distinguish final from initial particles; bars are used to distinguish summation variables.) In particular, since the left-hand side is independent of a^μ, so must be the right-hand side, and so the S -matrix vanishes unless the four-momentum is conserved. We can therefore write the part of the S -matrix that represents actual

interactions among the particles in the form:

$$S_{\beta\alpha} - \delta(\beta - \alpha) = -2\pi i M_{\beta\alpha} \delta^4 (p_\beta - p_x)$$

(Note: the amplitude $M_{\beta\alpha}$ itself contains terms that involve further delta function factors.)

Above equation should be regarded as a definition of what we mean by the Lorentz invariance of the S -matrix, rather than a theorem, because it is only for certain special choices of Hamiltonian that there exists a unitary operator that acts as in (2.23) on both 'in' and 'out' states.

2.3.9.2 Internal Symmetries

There are various symmetries, like the symmetry in nuclear physics under interchange of neutrons and protons, or the 'charge-conjugation' symmetry between particles and antiparticles, that have nothing directly to do with Lorentz invariance, and further appear the same in all inertial frames. Such a symmetry transformation T acts on the Hilbert space of physical states as a unitary operator $U(T)$, that induces linear transformations on the indices labelling particle species as

$$\begin{aligned} U(T)\Psi_{p_1\sigma_1 n_1; p_2\sigma_2 n_2, \cdots} = \sum_{\bar{n}_1 \bar{n}_2 \cdots} & \mathscr{D}_{\bar{n}_1 n_1}(T) \mathscr{D}_{\tilde{n}_2 n_2}(T) \cdots \\ & \times \Psi_{p_1\sigma_1 \bar{n}_1; p_2\sigma_2 \bar{n}_2; \cdots} \end{aligned} \tag{2.31}$$

In accordance with the general property of Transformation Group the $U(T)$ must satisfy the group multiplication rule

$$U(\bar{T})U(T) = U(\bar{T}T)$$

where $\bar{T}T$ is the transformation obtained by first performing the transformation T, then some other transformation $\vec{T}$. Acting on Eq. (2.31) with $U(\tilde{T})$, we see that the matrices $\mathscr{D}$ satisfy the same rule

$$\mathscr{D}(\bar{T})\mathscr{D}(T) = \mathscr{D}(\bar{T}T)$$

Finally, taking the scalar product of the states obtained by acting with $U(T)$ on one 'out' state and one 'in' state shows that $\mathscr{D}$ commutes with the S -matrix, in the sense that

$$\sum_{\bar{N}_1\bar{N}_2\cdots}\sum_{\tilde{N}_1'\bar{N}_2'\ldots}\mathscr{D}^*_{\bar{N}_1'n_1'}(T)\mathscr{D}^*_{\bar{N}_2'n_2'}(T)\mathscr{D}_{\bar{N}_1n_1}(T)\mathscr{D}_{\bar{N}_2n_2}(T)\cdots\times S_{p_1'\sigma_1'\bar{N}_1';p_2'\sigma_2'\bar{N}_2';\cdots,p_1\sigma_1\bar{N}_1;p_2\sigma_2\bar{N}_2;\cdots}$$

$$= S_{p_1'\sigma_1'n_1';p_2'\sigma_2'n_2';1\sigma_1n_1;p_2\sigma_2n_2,\cdots} \quad (2.32)$$

Again, this is a definition of what we mean by a theory being invariant under the internal symmetry T, because to derive Eq. (2.32) we still need to show that the same unitary operator $U(T)$ will induce the transformation (2.31) on both 'in' and 'out' states. This will be the case if there is an 'unperturbed' transformation operator $U_0(T)$ that induces these transformations on free-particle states,

$$U_0(T)\Phi_{p_1\sigma_1n_1:p_2\sigma_2n_2;\cdots} = \sum_{\bar{N}_1\bar{N}_2\ldots}\mathscr{D}_{\bar{N}_1n_1}(T)\mathscr{D}_{\bar{N}_2n_2}(T)\cdots\Phi_{p_1\sigma_1\bar{N}_1;p_2\sigma_2\bar{N}_2;\cdots}$$

and that commutes with both the free-particle and interaction parts of the Hamiltonian

$$U_0^{-1}(T)H_0U_0(T) = H_0$$
$$U_0^{-1}(T)VU_0(T) = V$$

From either the Lippmann-Schwinger equation (2.27) or from (2.28), we see that the operator $U_0(T)$ will induce the transformations (2.31) on 'in' and 'out' states as well as free-particle states, so that we can derive Eq. (2.31) taking $U(T)$ as $U_0(T)$.

A special case of great physical importance is that of a one-parameter Lie group, where T is a function of a single parameter θ, with

$$T(\bar{\theta})T(\theta) = T(\bar{\theta}+\theta)$$

In this case the corresponding Hilbert-space operators must take the form

$$U(T(0)) = \exp(iQ0)$$

with Q a Hermitian operator. Likewise the matrices $\partial(T)$ take the form

$$\mathscr{D}_{n'n}(T(\theta)) = \delta_{n'n} \exp(iq_n\theta)$$

where q_n are a set of real species-dependent numbers. Here Eq. (2.32) simply teils us that the q s are conserved: $S_{\beta\alpha}$ vanishes unless

$$q_{n'_1} + q_{n'_2} + \cdots = q_{n_1} + q_{n_2} + \cdots$$

The classic example of such a conservation law is that of conservation of Charge—(Which is an intrinsic property of any particle), its conservation denotes a specific case of conservation of Internal Symmetry.

2.3.9.3 Parity

To the extent that the symmetry under the transformation $\mathbf{x} \to -\mathbf{x}$ is really valid, there must exist a unitary operator P under which both 'in' and 'out' states transform as a direct product of single-particle states:

$$P\Psi^{\pm}_{p_1\sigma_1 n_1; p_2\sigma_2 n_2; \cdots} = \eta_{n_1}\eta_{n_2}\cdots\Psi_{\mathscr{P}p_1\sigma_1 n_1; \mathscr{P}p_2\sigma_2 n_2, \cdots}$$

where η_n is the intrinsic parity of particles of species n, and $\mathscr{P}$ reverses the space components of p^μ. (This is for massive particles; the modification for massless particles is obvious.) The parity conservation condition for the S -matrix is then:

$$\begin{aligned} S_{p'_1\sigma'_1 n'_1; p'_2\sigma'_2 n'_2; \cdots, p_1\sigma_1 n_1; p_2\sigma_2 n_2; \cdots} & \\ &= \eta^*_{n'_1}\eta^*_{n'_2}\cdots\eta_{n_1}\eta_{n_2}\cdots \\ &\times S_{\mathscr{P}p'_1\sigma'_1 n'_1; \mathscr{P}p'_2\sigma'_2 n'_2; \cdots, \mathscr{P}p_1\sigma_1 n_1; \mathscr{P}p_2\sigma_2 n_2; \cdots} \end{aligned}$$

Just as for internal symmetries, an operator P satisfying the Lorentz transformation of S-Matrix will actually exist if the operator P_0 which is defined to act this way on free-particle states commutes with V as well as H_0.

2.3.9.4 Time Reversal

It can be Proven that that the time-reversal operator T acting on a one-particle state $\Psi_{p,\sigma,n}$ gives a state $\Psi_{\mathscr{P}p,-\sigma,n}$ with reversed spin and momentum, times a phase $\zeta_n(-1)^{j-\sigma}$. A multi-particle state transforms as usual as a direct product of one-particle states, except that since this is a time-reversal transformation, we expect 'in' and 'out' states to be interchanged i,e

$$\mathrm{T}\Psi^{\pm}_{\vec{p}_1\sigma_1 n_1;p_2\sigma_2 n_2\cdots} = \zeta_{n_1}(-1)^{j_1-\sigma_1}\zeta_{n_2}(-1)^{j_2-\sigma_2}\cdots\Psi^{\mp}_{\mathscr{P}p_1(-\sigma_1)n_1;\mathscr{P}p_2(-\sigma_2)n_2,\ldots} \quad (2.33)$$

Above expression can be expressed in short hand notation as

$$T\Psi^{\pm}_{\alpha} = \Psi^{\mp}_{\mathscr{T}\alpha}$$

where $\mathscr{T}$ indicates a reversal of sign of three-momenta and spins as well as multiplication by the phase factors shown in Eq. (2.33). Because T is antiunitary, we have

$$\left(\Psi^{-}_{\beta},\Psi^{+}_{\alpha}\right) = \left(T\Psi^{+}_{\alpha},T\Psi^{-}_{\beta}\right)$$

so the time-reversal invariance condition for the S -matrix is

$$S_{\beta,\alpha} = S_{\mathscr{T}\alpha,\mathscr{T}\beta}$$

or in more detail

$$S_{p'_1\sigma'_1n'_1;p'_2\sigma'_2n'_2;\cdots,p_1\sigma_1n_1;p_2\sigma_2n_2;\cdots} = \zeta_{n'_1}(-1)^{j'_1-\sigma'_1}\zeta_{n'_2}(-1)^{j'_2-\sigma'_2}\cdots\zeta^{*}_{n_1}(-1)^{j_1-\sigma_1}\zeta^{*}_{n_2}(-1)^{j_2-\sigma_2}\cdots \times S_{\mathscr{P}p_1(-\sigma_1)n_1;\mathscr{P}p_2(-\sigma_2)n_2,\ldots\mathscr{P}p'_1(-\sigma'_1)n'_1;\mathscr{P}p'_2(-\sigma'_2)n'_2,\ldots}$$

Note that in addition to the reversal of momenta and spins, the role of initial and final states is interchanged, as would be expected for a symmetry involving the reversal of time.

The S -matrix will satisfy this transformation rule if the operator T_0 that induces time-reversal transformations on free-particle states

$$\mathrm{T}_0\Phi_{\alpha} \equiv \Phi_{\mathscr{T}\alpha}$$

commutes not only with the free-particle Hamiltonian (which is automatic) but also with the interaction:

$$\mathrm{T}_0^{-1} H_0 T_0 = H_0$$
$$\mathrm{T}_0^{-1} V T_0 = V$$

2.3.9.5 Charge Conjugation

As already mentioned, there is an internal symmetry transformation, known as charge-conjugation, which interchanges particles and antiparticles. Formally, this entails the existence of a unitary operator C, whose effect on multi-particle states is:

$$C\Psi^{\pm}_{p_1\sigma_1 n_1; p_2\sigma_2 n_2;\cdots} = \xi_{n_1}\xi_{n_2}\cdots\Psi^{\pm}_{p_1\sigma_1 n_1^c; p_2\sigma_2 n_2^c,\cdots} \tag{2.34}$$

where n^c is the antiparticle of particle type n, and ξ_n is yet another phase. If this is true for both 'in' and 'out' states then the S -matrix satisfies the invariance conditions

$$S_{p_1',\sigma_1' n_1'; p_2'\sigma_2' n_2';\cdots, p_1\sigma_1 n_1; p_2\sigma_2 n_2;\cdots} = (\xi^*_{n_1}\xi^*_{n_2}\cdots\xi_{n_1}\xi_{n_2}\cdots) S_{p_1'\sigma_1' n_1^{c\prime}; p_2'\sigma_2' n_2^{c\prime},\cdots p_1\sigma_1 n_1^c; p_2\sigma_2 n_2^c,\cdots}$$

As with other internal symmetries, the S -matrix will satisfy this condition if the operator C_0 that is defined to act as stated in Eq. (2.34) on freeparticle states commutes with the interaction V as well as H_0; in this case, we take $C = C_0$

2.3.10 S-Matrix as a tool to find Transition/Decay rates and cross sections

The S -matrix $S_{\beta\alpha}$ is the probability amplitude for the transition $\alpha \to \beta$, but what does this have to do with the transition rates and cross-sections measured by experimentalists? In particular,

$$S_{\beta\alpha} - \delta(\beta - \alpha) = -2\pi i M_{\beta\alpha}\delta^4(p_\beta - p_x)$$

shows that $S_{\beta\alpha}$ has a factor $\delta^4(p_\beta - p_x)$, which ensures the conservation of the total energy and momentum, so what are we to make of the factor $[\delta^4(p_\beta - p_\alpha)]^2$ in the transition probability $|S_{\beta\chi}|^2$? The proper way to approach these problems is by studying

the way that experiments are actually done, using wave packets to represent particles localized far from each other before a collision, and then following the time-history of these superpositions of multi-particle states. In what follows we will instead give a quick and easy derivation of the main results, actually more a mnemonic than a derivation, with the excuse that no interesting open problems in physics hinge on getting the fine points right regarding these matters.

We consider our whole system of physical particles to be enclosed in a large box with a macroscopic volume V. For instance, we can take this box as a cube, but with points on opposite sides identified, so that the single-valuedness of the spatial wave function requires the momenta to be quantized

$$\mathbf{p} = \frac{2\pi}{L}\,(n_1, n_2, n_3)$$

where the n_i are integers, and $L^3 = V$. Then all three-dimensional deltafunctions become

$$\delta_V^3\,(\mathbf{p}' - \mathbf{p}) \equiv \frac{1}{(2\pi)^3}\int_V d^3x e^{i(\mathbf{p}-\mathbf{p}')\mathbf{x}} = \frac{V}{(2\pi)^3}\delta_{\mathbf{p}',\mathbf{p}},$$

where $\delta_{\mathbf{p}',\mathbf{p}}$ is an ordinary Kronecker delta symbol, equal to one if the subscripts are equal and zero otherwise. The normalization condition (2.24) thus implies that the states we have been using have scalar products in a box which are not just sums of products of Kronecker deltas, but also contain a factor $[V/(2\pi)^3]^N$, where N is the number of particles in the state. To calculate transition probabilities we should use states of unit norm, so let us introduce states normalized approximately for our box

$$\Psi_\alpha^{\text{Box}} \equiv \left[(2\pi)^3/V\right]^{N_\alpha/2}\Psi_\alpha \tag{2.35}$$

with norm

$$\left(\Psi_\beta^{\text{Box}}\,,\Psi_\alpha^{\text{Box}}\right) = \delta_{\beta\alpha}$$

where $\delta_{\beta\alpha}$ is a product of Kronecker deltas, one for each three-momentum, spin, and species label, plus terms with particles permuted. Correspondingly, the S-matrix may be written

$$S_{\beta\alpha} = \left[\boldsymbol{V}/(2\pi)^3\right]^{\left(N_\beta+N_\alpha\right)/2} S_{\beta\alpha}^{\text{Box}},$$

where $S_{\beta\alpha}^{\text{Box}}$ is calculated using the states in equation (2.35). Of course, if we just leave our particles in the box forever, then every possible transition will occur again and

again. To calculate a meaningful transition probability we also have to put our system in a 'time box'. We suppose that the interaction is turned on for only a time T. One immediate consequence is that the energy-conservation delta function is replaced with

$$\delta_T\left(E_\alpha - E_\beta\right) = \frac{1}{2\pi}\int_{-T/2}^{T/2} \exp\left(i\left(E_\alpha - E_\beta\right)t\right) dt$$

The probability that a multi-particle system, which is in a state α before the interaction is turned on, is found in a state β after the interaction is turned off, is

$$P(\alpha \to \beta) = \left|S_{\beta\alpha}^{\text{Box}}\right|^2 = \left[(2\pi)^3/V\right]^{\left(N_\alpha + N_\beta\right)} \left|S_{\beta\alpha}\right|^2$$

This is the probability for a transition into one specific box state β. The number of one-particle box states in a momentum-space volume d^3p is $Vd^3p/(2\pi)^3$, because this is the number of triplets of integers n_1, n_2, n_3 for which the momentum

$$\mathbf{p} = \frac{2\pi}{L}\left(n_1, n_2, n_3\right)$$

lies in the momentum-space volume d^3p around p. We shall define the final-state interval $d\beta$ as a product of $d^3\mathbf{p}$ for each final particle, so the total number of states in this range is

$$d\mathcal{N}_\beta = \left[V/(2\pi)^3\right]^{N_f} d\beta$$

Hence the total probability for the system to wind up in a range $d\beta$ of final states is

$$dP(\alpha \to \beta) = P(\alpha \to \beta) d\mathcal{N}_\beta = \left[(2\pi)^3/V\right\}^{N_\alpha} \left|S_{\beta_\alpha}\right|^2 d\beta \tag{2.36}$$

We will restrict our attention throughout this section to final states β that are not only different (however slightly) from the initial state α, but that also satisfy the more stringent condition, that no subset of the particles in the state β (other than the whole state itself) has precisely the same four-momentum as some corresponding subset of the particles in the state α ,this means that we are considering only the connected part of the S-matrix.) For such states, we may define a delta function-free matrix element $M_{\beta\alpha}$:

$$S_{\beta\alpha} \equiv -2i\pi\delta_V^3\left(\mathbf{p}_\beta - \mathbf{p}_x\right)\delta_T\left(E_\beta - E_\alpha\right) M_{\beta\alpha}$$

Our introduction of the box allows us to interpret the squares of delta functions in

$|S_{\beta\alpha}|^2$ for $\beta \neq \alpha$ as

$$\left[\delta_V^3\left(\mathbf{p}_\beta - \mathbf{p}_\alpha\right)\right]^2 = \delta_V^3\left(\mathbf{p}_\beta - \mathbf{p}_\alpha\right)\delta_V^3(0) = \delta_V^3\left(\mathbf{p}_\beta - \mathbf{p}_\alpha\right)V/(2\pi)^3$$
$$\left[\delta_T\left(E_\beta - E_\alpha\right)\right]^2 = \delta_T\left(E_\beta - E_\alpha\right)\delta_T(0) = \delta_T\left(E_\beta - E_\alpha\right)T/2\pi$$

so Eq. (2.36) gives a differential transition probability

$$\begin{aligned} dP(\alpha \to \beta) =& (2\pi)^2\left[(2\pi)^3/V\right]^{N_\alpha - 1}(T/2\pi)\left|M_{\beta\alpha}\right|^2 \\ & \times \delta_V^3\left(\mathbf{p}_\beta - \mathbf{p}_\alpha\right)\delta_T\left(E_\beta - E_\alpha\right)d\beta \end{aligned}$$

If we let V and T be very large, the delta function product here may be interpreted as an ordinary four-dimensional delta function $\delta^4\left(p_\beta - p_\alpha\right)$. In this limit, the transition probability is simply proportional to the time T during which the interaction is acting, with a coefficient that may be interpreted as a differential transition rate:

$$\begin{aligned} d\Gamma(\alpha \to \beta) \equiv& dP(\alpha \to \beta)/T \\ =& (2\pi)^{3N_\alpha - 2}V^{1-N_\alpha}\left|M_{\beta\alpha}\right|^2\delta^4\left(p_\beta - p_\alpha\right)d\beta \end{aligned} \tag{2.37}$$

where now

$$S_{\beta\alpha} \equiv -2\pi i\delta^4\left(p_\beta - p_x\right)M_{\beta\alpha} \tag{2.38}$$

This is the master formula which is used to interpret calculations of $S-$ matrix elements in terms of predictions for actual experiments. We will come back to the interpretation of the factor $\delta^4\left(p_\alpha - p_\beta\right)d\beta$ later in this section. There are two cases of special importance:

$N_\alpha = 1$:

Here the volume V cancels in Eq. (2.37), which gives the transition rate for a single-particle state α to decay into a general multi-particle state β as

$$d\Gamma(\alpha \to \beta) = 2\pi\left|M_{\beta\alpha}\right|^2\delta^4\left(p_\beta - p_\alpha\right)d\beta$$

Of course, this makes sense only if the time T during which the interaction acts is much less than the mean lifetime τ_α of the particle α, so we cannot pass to the limit $T \to \infty$ in $\delta_T\left(E_\alpha - E_\beta\right)$. There is an unremovable width $\triangle E \simeq 1/T1/\tau_\alpha$ in this delta function, so above equation is only useful if the total decay rate $1/\tau_\alpha$ is much less than any of the characteristic energies of the process.

$N_a = 2$:

Here the rate (2.37) is proportional to $1/V$, or in other words, to the density of either particle at the position of the other one. Experimentalists generally report not the transition rate per density, but the rate per flux, also known as the cross-section. The flux of either particle at the position of the other particle is defined as the product of the density $1/V$ and the relative velocity u_α :

$$\Phi_\alpha = u_\alpha / V$$

(A general definition of u_α is given below; for the moment we will content ourselves with specifying that if either particle is at rest then u_x is defined as the velocity of the other.) Thus the differential cross-section is

$$d\sigma(\alpha \to \beta) \equiv d\Gamma(\alpha \to \beta)/\Phi_\alpha = (2\pi)^4 u_\alpha^{-1} \left|M_{\beta\alpha}\right|^2 \delta^4 \left(p_\beta - p_\alpha\right) d\beta$$

Even though the cases $N_\alpha = 1$ and $N_\alpha = 2$ are the most important, transition rates for $N_\alpha \geq 3$ are all measurable in principle, and some of them are very important in chemistry, astrophysics, etc. (For instance, in one of the main reactions that release energy in the sun, two protons and an electron turn into a deuteron and a neutrino.) subsection 2.3.11.2 presents an application of the master transition rate formula (2.37) for general numbers N_α of initial particles.

2.3.11 Unitarity Of S-Matrix in Canonical QFT's and Implications

In elementary particle physics, the S -matrix plays a fundamental role for describing scattering processes. In what follows, we want to describe the basic ideas of this fundamental concept in terms of a complex finite-dimensional Hilbert space X which has the dimension $N = 1, 2, \ldots$ Suppose that the two systems

$$\varphi_1, \ldots \varphi_N \text{ and } \psi_1, \ldots, \psi_N$$

form an orthonormal basis of the Hilbert space X. By the Dirac calculus, we get the following key relation:

$$\sum_{r=1}^{N} \langle \psi_j \mid \varphi_r \rangle \langle \varphi_r \mid \psi_k \rangle = \langle \psi_j \mid \psi_k \rangle = \delta_{jk}, \quad j, k = 1, \ldots, N$$

S -matrix. By definition, the transition amplitude from the state ψ_k to the state φ_j reads as

$$s_{jk} := \langle \varphi_j \mid \psi_k \rangle, \quad j, k = 1, \ldots, N$$

The idea is to regard this system (s_{jk}) of transition amplitudes as the elements of a complex $(N \times N)$ -matrix called the S -matrix as we have seen in subsection 2.3.4. From above equation we obtain immediately the following crucial property that The S -matrix (s_{jk}) must unitary. Explicitly,

$$\sum_{r=1}^{N} s_{rj}^{\dagger} s_{rk} = \delta_{jk}, \quad j, k = 1, \ldots, N$$

Transition probabilities. Letting $j = k$, we get

$$\sum_{r=1}^{N} |s_{rk}|^2 = 1, \quad k = 1, \ldots, N$$

This allows us the following interpretation. For given fixed state ψ_k with $k = 1, \ldots, N$, the number

$$|s_{rk}|^2 = |\langle \varphi_r \mid \psi_k \rangle|^2, \quad r = 1, \ldots, N$$

is the transition probability from the state ψ_k to the state φ_r. We now want to show that precisely unitary operators are related to systems of transition probabilities.

From transition probabilities to unitary operators: Let $\varphi_1, \ldots, \varphi_N$ and $\psi_1, \ldots, \psi_N$ be chosen as above. Define a linear operator $S : X \to X$ by setting

$$S\varphi_k := \psi_k, \quad k = 1, \ldots, N$$

Then, the operator S is unitary, that is,

$$\langle S\varphi \mid S\psi \rangle = \langle \varphi \mid \psi \rangle \quad \text{for all} \quad \varphi, \psi \in X$$

Note first that

$$\langle S\varphi_j \mid S\varphi_l \rangle = \langle \psi_j \mid \psi_l \rangle = \delta_{jl} \quad j, l = 1, \ldots, N$$

Thus, it follows from $\varphi = \sum_{k=1}^{N} \langle \varphi_k \mid \varphi \rangle \varphi_k$ and $\psi = \sum_{l=1}^{N} \langle \varphi_l \mid \psi \rangle \varphi_l$ that $\langle S\varphi \mid S\psi \rangle$ is equal to

$$\sum_{k,l=1}^{N} \langle \varphi_k \mid \varphi \rangle^{\dagger} \langle \varphi_l \mid \psi \rangle \langle S\varphi_k \mid S\varphi_l \rangle = \sum_{k=1}^{N} \langle \varphi \mid \varphi_k \rangle \langle \varphi_k \mid \psi \rangle = \langle \varphi \mid \psi \rangle$$

From unitary operators to transition probabilities: Conversely, suppose that we are given a linear unitary operator $S : X \to X$. Let $\varphi_1, \ldots, \varphi_N$ be an orthonormal basis of X. Finally, set

$$\psi_k := S\varphi_k, \quad k = 1, \ldots, N$$

Then, the system $\psi_1, \ldots, \psi_N$ is also an orthonormal basis. In fact,

$$\langle \psi_k \mid \psi_l \rangle = \langle S\varphi_k \mid S\varphi_l \rangle = \langle \varphi_k \mid \varphi_l \rangle = \delta_{jk}$$

The matrix elements of the operator S are given by

$$s_{jk} := \langle \varphi_j \mid S\varphi_k \rangle, \quad j, k = 1, \ldots, N$$

Hence $s_{jk} = \langle \varphi_j \mid \psi_k \rangle$, showing us that s_{jk} represents a transition probability, as in above expression.

Physical interpretation. Suppose that the following situation is met. - The given quantum system is in one of the states $\varphi_1, \ldots, \varphi_N$ at the initial time t_{in} . - The initial

state φ_k passes over to the state $S\varphi_k$ at the final time t_{out} .

Then, the real number

$$|s_{jk}|^2 = |\langle \varphi_j \mid S\varphi_k \rangle|^2$$

represents the transition probability of the quantum system from the initial state φ_k to the final state φ_j during the time interval $[t_{\text{in}}\,, t_{\text{out}}\,]$. It is crucial that the operator S is unitary. Otherwise, an interpretation in terms of transition probabilities is not possible.

Typically, the original S -matrix constructed in the Standard Model in particle physics is not unitary. However, this shortcoming can be fixed by introducing ghosts and antighosts.

2.3.11.1 Proof of Unitarity of S-Matrix in Canonical formalism

1.Unitarity of the Analaytical form : Recall that the completeness of in-out states relation states

$$\Psi = \int d\alpha \, |\Psi_\alpha\rangle \, \langle \Psi_\alpha \mid \Psi \rangle$$

and the requirement of in-out states is that they should be a energy eigenstates satisfying the Schrodinger equation

$$H\Psi_\alpha = E_\alpha \Psi_\alpha$$

with

$$E_\alpha = p_1^0 + p_2^0 + p_3^0 + \dots .$$

where p_1^o, p_2^o..are energies of single particles and E is the sum of all single particle energies. The Hamiltonian can be split into two parts as

$$H = H_0 + H_I$$

Where H_0 is the free Hamiltonian satisfied by

$$H_0\Phi_\alpha = E_\alpha \Phi_\alpha \tag{2.39}$$

and Φ_α has the same appearance as in-out states as discussed in section 2.3.6 and they are orthonormal as

$$\langle \Phi_\alpha \mid \Phi_\beta \rangle = \delta(\alpha - \beta)$$

or

$$\langle \Phi_{\alpha'} \mid \Phi_\alpha \rangle = \delta\left(\alpha' - \alpha\right)$$

The in-out states are defined as eigenstates of total Hamiltonian H

$$H = H_0 + H_I$$

i,e

$$H\Psi_\alpha^\pm = E_\alpha \Psi_\alpha^\pm$$

and they satisfy the equation

$$\int d\alpha e^{-iE_\alpha \tau} g(\alpha) \Psi_\alpha^\pm \longrightarrow \int d\alpha e^{-iE_\alpha \tau} g(\alpha) \Phi_\alpha$$

$\tau \longrightarrow -\infty, \tau \longrightarrow +\infty$(free states in long past and long future) and

$$e^{(-iH\tau)} \int d\alpha g(\alpha) \Psi_\alpha^\pm \longrightarrow e^{(-iH_0\tau)} \int d\alpha g(\alpha) \Phi_\alpha$$

for $\tau \to -\infty, \tau \to +\infty$

Hence

$$\Psi^\pm = \Omega(\pm\infty)\Phi_\alpha$$

where

$$\Omega(\pm\infty) = e^{(+iH\tau)} e^{(-iH_0\tau)}$$

Also

$$\left(\Psi_\beta^\pm, \Psi_\alpha^\pm\right) = (\Phi_\beta, \Phi_\alpha) = \delta(\beta - \alpha)$$

since

$$H\Psi_\alpha^\pm = E_\alpha \Psi_\alpha^\pm$$

$$\implies (H_0 + H_I)\Psi_\alpha^\pm = E_\alpha \Psi_\alpha^\pm$$

$$\implies H_0\Psi_\alpha^\pm - E_\alpha \Psi_\alpha^\pm = -H_I \Psi_\alpha^\pm$$

Or

$$(E_\alpha - H_0)\Psi_\alpha^\pm = H_I \Psi_\alpha^\pm$$

and formal solution of this will be

$$\Psi_\alpha^\pm = \Phi_\alpha + (E_\alpha - H_0 \pm i\epsilon)^{-1} H_I \Psi_\alpha^\pm$$

In Dirac notation

$$\left|\Psi_\alpha^\pm\right\rangle = |\Phi_\alpha\rangle + (E_\alpha - H_0 \pm i\epsilon)^{-1} H_I \left|\Psi_\alpha^\pm\right\rangle$$

Inserting the completeness relation

$$\int d\beta |\Phi_\beta\rangle\langle\Phi_\beta| = 1$$

$$\implies |\Psi_\alpha^\pm\rangle = |\Phi_\alpha\rangle + \int d\beta |\Phi_\beta\rangle\langle\Phi_\beta| (E_\alpha - H_0 \pm i\epsilon)^{-1} H_I |\Psi_\alpha^\pm\rangle$$

$$\implies |\Phi_\alpha\rangle + \int d\beta \, |\Phi_\beta\rangle \frac{1}{(E_\alpha - E_\beta \pm i\epsilon)} \left\langle \Phi_\beta \right| H_I \left| \Psi_\alpha^\pm \right\rangle$$

$$\implies |\Phi_\alpha\rangle + \int d\beta \frac{T_{\beta\alpha}^\pm}{(E_\alpha - E_\beta \pm i\epsilon)} |\Phi_\beta\rangle$$

where

$$T_{\beta\alpha}^\pm = \langle\Phi_\beta| H_I |\Psi_\alpha^\pm\rangle$$

In-state particle content = state α; at $t = -\infty$ and out state particle content = state β at ; $t = +\infty$ Now the S-Matrix is denoted by

$$S_{\beta\alpha} = \left\langle \Psi_\beta^- \mid \Psi_\alpha^+ \right\rangle$$

now we can see

$$\int d\beta S_{\beta\gamma}^* S_{\beta\alpha} = \int d\beta \langle \Psi_\beta^- \left| \Psi_\gamma^+ \right\rangle^* \left\langle \Psi_\beta^- \mid \Psi_\alpha^+ \right\rangle$$

$$\Rightarrow \int d\beta \langle \Psi_\gamma^+ | \Psi_\beta^- \rangle \langle \Psi_\beta^- \mid \Psi_\alpha^+ \rangle = \langle \Psi_\gamma^+ \int d\beta \mid \Psi_\beta^- \rangle \langle \Psi_\beta^- | \Psi_\alpha^+ \rangle = \left\langle \Psi_\gamma^+ | \Psi_\alpha^+ \right\rangle$$

since

$$\langle \Psi_\beta^\pm | \Psi_\alpha^\pm \rangle = \delta(\beta - \alpha)$$

hence $\Rightarrow \langle \Psi_y^+ \Psi_\alpha^+ \rangle = \delta(\gamma - \alpha)$ and finally we get

$$\int d\beta S_{\beta\gamma}^* S_{\beta\alpha} = \delta(\gamma - \alpha) \Rightarrow S^\dagger S = 1$$

Similarly if

$$\int d\beta S_{\gamma\beta} S_{\alpha\beta}^* = \delta(\gamma - \alpha) \Rightarrow S S^\dagger = 1$$

Proof: According to Born approximation

$$S_{\beta\alpha} = \delta(\beta - \alpha) - 2\pi i \delta\left(E_\alpha - E_\beta\right) T_{\beta\alpha}^+$$

where

$\delta\left(E_\alpha - E_\beta\right)$ = Energy conserving delta function

$\delta(\beta - \alpha)$ =Trivial amplitude factor

and $T_{\beta\alpha}^+ = \langle \Phi_\beta | H_I | \Psi_\alpha^+ \rangle$

Actually for Born approximation

$$S_{\beta\alpha} \approx \delta(\beta - \alpha) - 2\pi i \delta\left(E_\alpha - E_\beta\right) \langle \Phi_\beta | H_I | \Phi_\alpha \rangle$$

i,e $|\Psi_\alpha^+\rangle \approx |\Phi_\alpha\rangle$(approximated as free particle state).

Now consider the Most general Matrix element given by

$$\left\langle \Psi_\beta^\pm \left| H_I \right| \Psi_\alpha^\pm \right\rangle$$

Recall we had

$$|\Psi_\alpha^\pm\rangle = |\Phi_\alpha\rangle + (E_\alpha - H_0 \pm i\epsilon)^{-1} H_I |\Psi_\alpha^\pm\rangle$$

then

$$\left\langle \Psi_\beta{}^{\pm}\right| = \langle \Phi_\beta| + \left\langle \Psi_\beta^{\pm}\right| \left(E_\beta - H_0 \pm i\epsilon\right)^{-1} H_I^*$$

since

$$\left\langle \Psi_\beta{}^{\pm} \left| H_I \right| \Psi_\alpha{}^{\pm} \right\rangle = \left\langle \Psi_\beta{}^{\pm} \left| H_1 \right| \Psi_\alpha^{\pm} \right\rangle$$

hence putting the expressions for $|\Psi_\alpha^{\pm}\rangle$ and $\langle \Psi_\beta{}^{\pm}|$ we get

$$\left\langle \Phi_\beta{}^{\pm} \left| H_1 \left(|\Phi_\alpha\rangle + \left(E_\alpha - H_0 \pm i\epsilon\right)^{-1} H_I \left| \Psi_\alpha^{\pm} \right\rangle \right) \right. = (\langle \Phi_\beta| + \langle \Psi_\beta^{\pm}|(E_\beta - H_0 \pm i\epsilon^{-1} H_1^*) H_1 \Psi_\alpha^{\pm}\rangle$$

$$\begin{aligned} &\Longrightarrow \langle \Psi_\beta \pm |H_1| \Phi_\alpha\rangle + \left\langle \Psi_\beta^{\pm} \left| H_I \left(E_\alpha - H_0 \pm i\epsilon\right)^{-1} H_I \right| \Psi_\alpha^{\pm} \right\rangle \\ &= \langle \Phi_\beta \left| H_I \right| \Psi_\alpha \pm\rangle + \left\langle \Phi_\beta{}^{\pm} \left| \left(E_\beta - H_0 \pm i\epsilon\right)^{-1} H_2^* \right| H_I \Psi_\alpha \pm \right\rangle Now we have (2.40) \end{aligned}$$

$$= \frac{\left\langle \Psi_\beta^{\pm} \left| H_I H_I \right| \Psi_\alpha^{\pm} \right\rangle}{\left(E_\alpha - H_0 \pm i\epsilon\right)} + \frac{\langle \Psi_\beta \pm H_I{}^* H_I \Psi_\alpha^{\pm}\rangle}{\left(E_\beta - H_0 \pm i\epsilon\right)}$$

Summing over complete Set of $|\Phi_y\rangle$ states we get

$$\int d\gamma |\Phi_\gamma\rangle\langle\Phi_\gamma| = 1$$

$$T_{\alpha\beta}^{*\pm} - T_{\beta\alpha}^{\pm} = \frac{-\left\langle \Psi_\beta^{\pm} \left| H_I \int d\gamma \right| \Phi_\gamma \right\rangle \left\langle \Phi_\gamma \left| H_I \right| \Psi_\alpha^{\pm} \right\rangle}{\left(E_\alpha - E_\gamma \pm i\epsilon\right)} + \frac{\left\langle \Psi_\beta{}^{\pm} H_I^* \int d\gamma \mid \Phi_\gamma \right\rangle \left\langle \Phi_\gamma \mid H_I \Psi_\alpha^{\pm} \right\rangle}{\left(E_\beta - E_\gamma \pm i\epsilon\right)}$$

$$\Rightarrow \frac{-\int d\gamma \left\langle \Psi_\beta^{\pm} \mid H_I \Phi_\gamma \right\rangle \left\langle \Phi_\gamma \mid H_I \Psi_\alpha^{\pm} \right\rangle}{\left(E_\alpha - E_\gamma \pm i\epsilon\right)} + \frac{\int d\gamma \left\langle \Psi_\beta^{\pm} H_I^* \Phi_\gamma \right\rangle \left\langle \Phi_\gamma \mid H_I \Psi_\alpha^{\pm} \right\rangle}{\left(E_\beta - E_\gamma \pm i\epsilon\right)}$$

$$\Rightarrow - \int d\gamma \frac{T_{\gamma\beta}^{*\pm} \quad T_{\gamma\alpha}^{\pm}}{\left(E_\alpha - E_\gamma \pm i\epsilon\right)} + \int d\gamma \frac{T_{\gamma\beta}^{*\pm} \quad T_{\gamma\alpha}^{\pm}}{\left(E_\beta - E_\gamma \pm i\epsilon\right)}$$

or

$$\begin{aligned} T_{\alpha\beta}^{*\pm} - T_{\beta\alpha}^{*\pm} = &- \int d\gamma \;\; T_{\gamma\beta}^{*\pm} \;\; T_{\gamma\alpha}^{*\pm} \\ &\times \left(\left[E_\alpha - E_\gamma \pm i\epsilon\right]^{-1} - \left[E_\beta - E_\gamma \mp i\epsilon\right]^{-1} \right). \end{aligned} \tag{2.41}$$

To prove the orthonormality of the 'in' and 'out' states, divide by $E_\alpha - E_\beta \pm 2i\epsilon$. This

gives

$$\left(\frac{T^{\pm}_{\alpha\beta}}{E_\beta - E_\alpha \pm 2i\epsilon}\right)^{\star} + \frac{T^{\pm}_{\beta\alpha}}{E_\alpha - E_\beta \pm 2i\epsilon} = -\int d\gamma \left(\frac{T^{\pm}_{\gamma\beta}}{E_\beta - E_\alpha \pm i\epsilon}\right)^{\star} \frac{T_{\gamma\alpha}\pm}{E_\alpha - E_\beta \pm i\epsilon}$$

The 2ϵs in the denominators on the left-hand side can be replaced with ϵs, since the only important thing is that these are positive infinitesimals. We see then that $\delta(\beta - \alpha) + T^{\pm}_{\beta\alpha}/\left(E_\beta - E_\alpha \pm i\epsilon\right)$ is unitary. With Lippmann Schwinger Equation(2.28), this is just the statement that the $\Psi^{\pm}_{\alpha}$ form two orthonormal sets of state-vectors.

The unitarity of the S-matrix can be proved in a similar fashion by multiplying (2.41) with $\delta\left(E_\beta - E_\alpha\right)$ instead of $\left(E_\alpha - E_\beta \pm 2i\epsilon\right)^{-1}$.

Multiplying both sides by $\delta\left(E_\beta - E_\alpha\right)$

$$\begin{aligned} T^{*\pm}_{\alpha\beta}\delta\left(E_\beta - E_\alpha\right) - T^{\pm}_{\beta\alpha}\delta\left(E_\beta - E_\alpha\right) = &\int d\gamma \frac{T^{*\pm}_{\gamma\beta}\ \ T^{\pm}_{\gamma\alpha}\delta\left(E_\beta - E_\alpha\right)}{\left(E_\alpha - E_\gamma \pm i\epsilon\right)} \\ &+ \int d\gamma \frac{T^{*\pm}_{\gamma\beta}\ \ T^{\pm}_{\gamma\alpha}\delta\left(E_\beta - E_\alpha\right)}{\left(E_\beta - E_\gamma \pm i\epsilon\right)} \end{aligned} \tag{2.42}$$

Since according to born approximation

$$S_{\beta\alpha} = \delta(\beta - \alpha) - 2\pi i\delta\left(E_\alpha - E_\beta\right) T^{+}_{\beta\alpha}$$

Grouping the terms with similar coefficients we finally get

$$\int d\beta S^{*}_{\beta\gamma} S_{\beta\alpha} = \delta(\gamma - \alpha) \Rightarrow S^{\dagger}S = 1$$

Hence S -Matrix is always Unitary

2.Unitarity of the Perturbative/Dyson Series form : In section 2.3.1 we have derived the perturbative form of S-matrix as Dyson series expansion , which is given as

$$S_n = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 ... \int_{-\infty}^{t_\infty} dt_n \mathcal{T}[H_I(t_1)...H_I(t_n)] \tag{2.43}$$

Where $H_I(t_n)$ is the Interacting Hamiltonian .We convert this into Hamiltonian Density ,since $\mathcal{H}_I(t_n)$ is more useful in field theory.

In terms of Hamiltonian Density we have

$$H_I(t_n) = \int d^3x_n \mathcal{H}_I(t_n)$$

Hence the expansion becomes

$$S_n = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} d^4x_1 ... \int_{-\infty}^{t_\infty} d^4x_n \mathcal{T}[\mathcal{H}_I(t_1)\mathcal{H}_I(t_2)...\mathcal{H}_I(t_n)] \tag{2.44}$$

where $\mathcal{T}[\mathcal{H}_I(t_1)\mathcal{H}_I(t_2)...\mathcal{H}_I(t_n)]$ denotes the Time ordered product of the Interacting Hamiltonian described at different point in time and here $t_1 > t_2 > t_3 ... > t_n$.

Now we have already described that for a theory to be renormalizable , the interacting part cannot be more that ϕ^4 in terms of field variable. Since the typical interacting Hamiltonian already has a certain ϕ^2 term, hence in the integral

$$\int_{-\infty}^{t_\infty} d^4x_n \mathcal{T}[\mathcal{H}_I(t_1)\mathcal{H}_I(t_2)]$$

only 2 terms of $\mathcal{H}_I(t_1).\mathcal{H}_I(t_2)$ suffices. Since the value of coupling constant which is denoted as λ and for a typical $\mathcal{H}_I(t)$ it becomes

$$\mathcal{H}_I(t) = \lambda\phi^2 \quad \text{or} \quad \lambda\phi^4$$

Then,

$$\mathcal{H}_I(t_1).\mathcal{H}_I(t_2) \approx \lambda^2$$

which is smaller than λ.

Similarly for three terms

$$\mathcal{H}_I(t_1).\mathcal{H}_I(t_2)\mathcal{H}_I(t_3) \approx \lambda^3$$

which is very small compared toλ.

Hence, we will consider upto the 2nd order terms of S-Matrix expansion. We have

$$S_n = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} d^4x_1 ... \int_{-\infty}^{t_\infty} d^4x_n \mathcal{T}[\mathcal{H}_I(t_1)\mathcal{H}_I(t_2)] \tag{2.45}$$

If we expand the individual order term as

$$S_n = I - i\int_{-\infty}^{\infty} \mathcal{H}_I d^4x_1 - \frac{1}{2}\int_{-\infty}^{t_\infty}\int_{-\infty}^{t_\infty} \mathcal{T}[\mathcal{H}_I(t_1)\mathcal{H}_I(t_2)]d^4x_1 d^4x_2 + .. \tag{2.46}$$

Therefore

$$S = S^{(0)} + S^{(1)} + S^{(2)} + ... = \sum_{n=0}^{\infty} S^{(n)} \tag{2.47}$$

We take only upto 2nd order ,hence

$$S = S^{(0)} + S^{(1)} + S^{(2)} \tag{2.48}$$

also,

$$S^\dagger = S^{\dagger(0)} + S^{\dagger(1)} + S^{\dagger(2)} \tag{2.49}$$

For Unitarity $S^\dagger S = 1 = SS^\dagger$ then

$$\begin{aligned} S^\dagger S &\approx \left[S^{\dagger(0)} + S^{\dagger(1)} + S^{\dagger(2)}\right]\left[S^{(0)} + S^{(1)} + S^{(2)}\right] \\ &\approx S^{\dagger(0)}S^{(0)} + S^{\dagger(0)}S^{(1)} + S^{\dagger(0)}S^{(2)} + S^{\dagger(1)}S^{(0)} \\ &+ S^{\dagger(1)}S^{(1)} + S^{\dagger(1)}S^{(2)} + S^{\dagger(2)}S^{(0)} + S^{\dagger(2)}S^{(1)} + S^{\dagger(2)}S^{(2)} \end{aligned} \tag{2.50}$$

Hence,we get

$$S^\dagger S \approx 1 + S^{\dagger(0)}S^{(1)} + ... + S^{\dagger(2)}S^{(2)} \tag{2.51}$$

Since we already have 1, which implies that the higher order multiples must vanish.

Let us try to prove this by taking the most general last term $S^{\dagger(2)}S^{(2)}$ We have seen that how S-Matrix creates a asymptotic state ϕ_i in the long part $t = -\infty$ to another asymptotically free state ϕ_f in the long past. That is matrix elements of S can be written as

$$S_{fi} = \langle \phi_f | S | \phi_i \rangle$$

However there are infinitely many states between ϕ_i and ϕ_f. Now for unitarity of the S-Matrix, we have seen that in general for 2 intermediate steps say,

$$\sum_{r=1}^{\infty} S^{\dagger}_{rj} S_{rk} = \delta_{jk} \qquad j,k = 1..N$$

set j=k then

$$\sum_{r=1}^{\infty} S^{\dagger}_{rj} S_{rj} = 1$$

Let j=i(Initial state) and r=f(Final State) we get

$$\sum_{r=1}^{\infty} S^{\dagger}_{fi} S_{fi} = 1$$

Similarly we have

$$S_{fi} = \langle \phi_f | S | \phi_i \rangle$$

and

$$S^{\dagger}_{fi} = \langle \phi_i | S^{\dagger} | \phi_f \rangle$$

then we get

$$\sum_{i=1}^{\infty} S_{fi} S^{\dagger}_{fi} = 1$$

Hence

$$\sum_{i=1}^{\infty} \langle \phi_f | S | \phi_i \rangle \langle \phi_i | S^{\dagger} | \phi_f \rangle = 1 \tag{2.52}$$

$$\implies \langle \phi_f | S \sum_{i=1}^{\infty} | \phi_i \rangle \langle \phi_i | S^{\dagger} | \phi_f \rangle = 1 \tag{2.53}$$

By using completeness relation we can write

$$\sum_{i=1}^{\infty} | \phi_i \rangle \langle \phi_i = 1$$

so we can write

$$\langle \phi_f | S S^{\dagger} | \phi_f \rangle = 1 \tag{2.54}$$

Therefore we can say that,in the expansion of Dyson series

$$SS^{\dagger} \approx 1 + S^{(1)}S^{\dagger(0)} + ... + S^{(2)}S^{\dagger(2)} \tag{2.55}$$

all other terms must vanish(Except the 1st term),if the S-Matrix has to be Unitary.

For the last term we have

$$S^{(}2) = -\frac{1}{2!}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathcal{T}[\mathcal{H}_I(t_1)\mathcal{H}_I(t_2)]d^4x_1d^4x_2 \qquad t_1 > t_2 \tag{2.56}$$

$$S^{\dagger(2)} = -\frac{1}{2!}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathcal{T}[\mathcal{H}_I(t_1)\mathcal{H}_I(t_2)]^{\dagger}d^4x_1d^4x_2 \qquad t_1 > t_2 \tag{2.57}$$

$$\implies -\frac{1}{2!}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathcal{T}[\mathcal{H}_I^{\dagger}(t_2)\mathcal{H}_I^{\dagger}(t_1)]d^4x_1d^4x_2 \qquad t_1 > t_2 \tag{2.58}$$

Let $\mathcal{H}_I^{\dagger}(t_2) = A(x)$ and $\mathcal{H}_I^{\dagger}(t_1) = B(y)$, we already know that

$$\mathcal{T}[A(x)B(x)] = \Theta(x-y)A(x)B(y) \pm \Theta(y-x)B(y)A(x)$$

since $t_1 > t_2$,so $y > x$. Then only 2nd term survives.

$$\mathcal{T}[A(x)B(y)] = \Theta(y-x)B(y)A(x)$$

$$\mathcal{T}[\mathcal{H}_I^{\dagger}(t_2)\mathcal{H}_I^{\dagger}(t_1)] = \mathcal{H}_I^{\dagger}(t_1)\mathcal{H}_I^{\dagger}(t_2)$$

Then finally

$$S^{\dagger(2)} = -\frac{1}{2!}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}[\mathcal{H}_I^{\dagger}(t_1)\mathcal{H}_I^{\dagger}(t_2)]d^4x_1d^4x_2 \tag{2.59}$$

Put these in equation 2.50 and we get

$$\langle\phi_f|S^{(0)}S^{\dagger(0)} + ... + S^{(2)}S^{\dagger(2)}|\phi_f\rangle = 1 \tag{2.60}$$

$$\langle\phi_f|S^{(0)}S^{\dagger(0)}+...+(-\frac{1}{2!}\int_{-\infty}^{\infty}\mathcal{H}_I(t_1)\mathcal{H}_I(t_2)d^4x_1d^4x_2)(-\frac{1}{2!}\int_{-\infty}^{\infty}[\mathcal{H}_I^{\dagger}(t_1)\mathcal{H}_I^{\dagger}(t_2)]d^4x_1d^4x_2)|\phi_f\rangle = 1 \tag{2.61}$$

take the last term, that is $S^{\dagger(2)}|\phi_f\rangle$

$$-\frac{1}{2!}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathcal{H}_I^{\dagger}(t_1)d^4x_1\mathcal{H}_I^{\dagger}(t_2)d^4x_2)|\phi_f\rangle \tag{2.62}$$

$$-\frac{1}{2!}\int_{-\infty}^{\infty}\mathcal{H}_I^{\dagger}(t_1)d^4x_1\int_{-\infty}^{\infty}\mathcal{H}_I^{\dagger}(t_2)d^4x_2)|\phi_f\rangle \tag{2.63}$$

We know that in the interaction picture

$$\mathcal{H}(t)|\Psi(t)\rangle = i\hbar\frac{d}{dt}|\Psi(t)$$

then

$$-\frac{1}{2!}\int_{-\infty}^{\infty}\mathcal{H}_I^{\dagger}(t_1)d^4x_1\Big[\int_{-\infty}^{\infty}i\hbar\frac{d}{dt}|\phi_f\rangle d^4x_2\Big] \tag{2.64}$$

$$-\frac{1}{2!}\int_{-\infty}^{\infty}\mathcal{H}_I^{\dagger}(t_1)d^4x_1\Big[\int_{-\infty}^{\infty}i\hbar|\phi_f(\infty)\rangle - |\phi_f(-\infty)\rangle\Big] \tag{2.65}$$

since

$$|\phi_f(\infty)\rangle = |\phi_f\rangle \qquad |\phi_f(-\infty)\rangle = |\phi_f\rangle$$

Hence the above equation becomes zero. that is $S^{\dagger(2)}|\phi_f\rangle = 0$, so we can write $S^{(2)}S^{\dagger(2)}|\phi_f\rangle = 0$.

so in general we can write

$$S^{(n)}S^{\dagger(n)}|\phi_f\rangle = 0 \qquad (n = 1, 2, 3, ..)$$

we can conclude that only the zeroth order product survives,hence

$$\langle\phi_f|S^{(0)}S^{\dagger(0)}|\phi_f\rangle = 1 \tag{2.66}$$

$$\langle\phi_f|I|\phi_f\rangle = 1 \tag{2.67}$$

$$\langle\phi_f|\phi_f\rangle = 1 \tag{2.68}$$

Hence for $SS^{\dagger} = 1$

$$SS^{\dagger}|\phi_f\rangle = |\phi_f\rangle$$

$$SS^{\dagger} = I$$

2.3.11.2 Implication of Unitaritry of S-Matrix

A. Optical Theorem The unitarity of the S -matrix imposes an interesting and useful condition relating the amplitude $M_{\alpha\alpha}$ for forward scattering in an arbitrary

multiparticle state α to the total rate for all reactions in that state. Recall that in the general case, where the state β may or may not be the same as the state α, the S -matrix may be written as

$$S_{\beta\alpha} = \delta(\beta - \alpha) - 2\pi i\delta^4 (p_\beta - p_\alpha) M_{\beta x}$$

The unitarity condition $S^\dagger S = 1$ then gives

$$\begin{aligned}\delta(\gamma - \alpha) = \int d\beta S^*_{\beta\rangle} S_{\beta x} = \delta(\gamma - x) - 2\pi i\delta^4 (p_\gamma - p_x) M_{\gamma\alpha} \\ + 2\pi i\delta^4 (p_\gamma - p_x) M^*_{\alpha\rangle} + 4\pi^2 \int d\beta\delta^4 (p_\beta - p_\gamma) \delta^4 (p_\beta - p_\alpha) M^*_{\beta_\gamma} M_{\beta\alpha}\end{aligned}$$

Cancelling the term $\delta(\gamma - x)$ and a factor $2\pi\delta^4 (p_y - p_x)$, we find that for $p_\gamma = p_\alpha$

$$0 = -iM_{i\alpha} + iM^*_{\alpha_i} + 2\pi \int d\beta\delta^4 (p_\beta - p_\alpha) M^*_{\beta\gamma} M_{\beta\alpha}$$

This is most useful in the special case $\alpha = \gamma$, where it reads

$$\operatorname{Im} M_{\alpha\alpha} = -\pi \int d\beta\delta^4 (p_\beta - p_\alpha) |M_{\beta\alpha}|^2$$

Using the expression of differential transition rate i,e

$$\begin{aligned}d\Gamma(\alpha \to \beta) \equiv & dP(\alpha \to \beta)/T \\ & = (2\pi)^{3N_\alpha - 2} V^{1-N_\alpha} |M_{\beta\alpha}|^2 \delta^4 (p_\beta - p_\alpha) d\beta\end{aligned}$$

Using the expression for $\operatorname{Im} M_{\alpha\alpha}$ the above equation can be expressed as a formula for the total rate for all reactions produced by an initial state α in a volume V

$$\begin{aligned}\Gamma_\alpha &\equiv \int d\beta \frac{d\Gamma(\alpha \to \beta)}{d\beta} \\ &= (2\pi)^{3N_2 - 2} V^{1-N_2} \int d\beta\delta^4 (p_\beta - p_\alpha) |M_{\beta\alpha}|^2 \\ &= -\frac{1}{\pi} (2\pi)^{3N_\alpha - 2} V^{1-N_\alpha} \operatorname{Im} M_{\alpha\alpha}\end{aligned}$$

In particular, where α is a two-particle state, this can be written

$$\operatorname{Im} M_{x\alpha} = -u_\alpha \sigma_\alpha / 16\pi^3$$

where u_α is the relative velocity given by

$$u_\alpha = \sqrt{(p_1 \cdot p_2)^2 - m_1^2 m_2^2}/E_1 E_2$$

where p_1, p_2 and m_1, m_2 are the four-momenta and mass of the two particles in the initial state α. in state α, and σ_x is the total cross-section in this state, given by integrating

$$d\sigma(\alpha \to \beta) \equiv d\Gamma(\alpha \to \beta)/\Phi_\alpha = (2\pi)^4 u_\alpha^{-1} \left|M_{\beta\alpha}\right|^2 \delta^4 \left(p_\beta - p_\alpha\right) d\beta$$

hence

$$\sigma_\alpha \equiv \int d\beta d\sigma(\alpha \to \beta)/d\beta = (2\pi)^4 u_\alpha^{-1} \int d\beta \left|M_{\beta\alpha}\right|^2 \delta^4 \left(p_\beta - p_\alpha\right)$$

This is usually expressed in a slightly different way, in terms of a scattering amplitude $f(\alpha \to \beta)$. We know that the differential cross-section for two-body scattering in the center-of-mass frame is given by

$$\frac{d\sigma(x \to \beta)}{d\Omega} = \frac{(2\pi)^4 k' E_1' E_2' E_1 E_2}{k E^2} \left|M_{\beta\alpha}\right|^2$$

where k' and k are the magnitudes of the momenta in the initial and final states. We therefore define the scattering amplitude as

$$f(\alpha \to \beta) \equiv -\frac{4\pi^2}{E} \sqrt{\frac{k' E_1' E_2' E_1 E_2}{k}} M_{\beta\alpha}$$

so that the differential cross-section is simply

$$\frac{d\sigma(\alpha \to \beta)}{d\Omega} = |f(\alpha \to \beta)|^2.$$

In particular, for elastic two-body scattering, we have

$$f(\alpha \to \beta) \equiv -\frac{4\pi^2 E_1 E_2}{E} M_{\beta\alpha}$$

now we have seen that if α is a two-particle state, then

$$\operatorname{Im} M_{\alpha\alpha} = -u_\alpha \sigma_\alpha / 16\pi^3$$

if we take

$$f(\alpha \to \beta) \equiv -\frac{4\pi^2 E_1 E_2}{E} M_{\beta\alpha}$$

and put $f(\alpha \to \alpha)$ and take $\operatorname{Im} f(\alpha \to \alpha)$ we get

$$\operatorname{Im} f(\alpha \to \alpha) \equiv -\frac{4\pi^2 E_1 E_2}{E} \operatorname{Im} M_{\alpha\alpha}$$

$$\operatorname{Im} f(\alpha \to \alpha) \equiv -\frac{4\pi^2 E_1 E_2}{E} .(-u_\alpha \sigma_\alpha / 16\pi^3)$$

we now use the expression of relative velocity u_α given by

$$u_\alpha = \sqrt{(p_1 \cdot p_2)^2 - m_1^2 m_2^2}/E_1 E_2$$

For Simplicity if we work in the 'center-of-mass' frame, where the total three-momentum vanishes, we have

$$p_1 = (\mathbf{p}, E_1), \quad p_2 = (-\mathbf{p}, E_2)$$

and hence

$$u_\alpha = \frac{|\mathbf{p}|\,(E_1 + E_2)}{E_1 E_2}$$

puting this value of u_α in

$$\operatorname{Im} f(\alpha \to \alpha) = -\frac{4\pi^2 E_1 E_2}{E} .(-u_\alpha \sigma_\alpha / 16\pi^3)$$

finally we get

$$\operatorname{Im} f(\alpha \to \alpha) = \frac{k}{4\pi} \sigma_\alpha$$

Where k is the total magnitude of momentum of incoming particles in C.O.M frame.

This form of the unitarity condition is known as the **optical theorm**. There is a pretty consequence of the optical theorem that tells much about the pattern of scattering at high energy. The scattering amplitude f may be expected to be a smooth function of angle, so there must be some solid angle $\Delta\Omega$ within which $|f|^2$ has nearly the same value (say, within a factor 2) as in the forward direction. The total cross-section is then bounded by

$$\sigma_\alpha \geq \int |f|^2 d\Omega \geq \frac{1}{2} |f(\alpha \to \alpha)|^2 \Delta\Omega \geq \frac{1}{2} |\operatorname{Im} f(\alpha \to \alpha)|^2 \Delta\Omega$$

Using the optical theorm then yields an upper bound on $\Delta\Omega$

$$\Delta\Omega \leq 32\pi^2/k^2\sigma_\alpha$$

As we shall see in the next section, total cross-sections are usually expected to approach constants or grow slowly at high energy, so above equation shows that the solid angle around the forward direction within which the differential cross-section is roughly constant shrinks at least as fast as $1/k^2$ for $k \to \infty$. This increasingly narrow peak in the forward direction at high energies is known as a diffraction peak.

B. Boltzman H-theorem The same argument that led from the unitarity condition $S^\dagger S = 1$ to our result

$$\mathrm{Im}\, M_{\alpha\alpha} = -\pi \int d\beta \delta^4 (p_\beta - p_\alpha) \left|M_{\beta\alpha}\right|^2$$

also allows us to use the other unitarity relation $SS^\dagger = 1$ to derive another result

$$\mathrm{Im}\, M_{\alpha\alpha} = -\pi \int d\beta \delta^4 (p_\beta - p_\alpha) \left|M_{\alpha\beta}\right|^2$$

Putting these two equations then yields the reciprocity relation

$$\int d\beta \delta^4 (p_\beta - p_\alpha) \left|M_{\beta\alpha}\right|^2 = \int d\beta \delta^4 (p_\beta - p_\alpha) \left|M_{\alpha,\beta}\right|^2$$

or in other words

$$\int d\beta \frac{d\Gamma(\alpha \to \beta)}{d\beta} = \int d\beta \frac{d\Gamma(\beta \to \alpha)}{d\alpha}$$

This result can be used in deriving some of the most important results of kinetic theory. If $P_\alpha dx$ is the probability of finding the system in a volume $d\alpha$ of the space of multiparticle states Φ_α, then the rate of decrease in P_α due to transitions to all other states is $P_\alpha \int d\beta d\Gamma(\alpha \to \beta)/d\beta$, while the rate of increase of P_α due to transitions from all other states is $\int d\beta P_\beta d\Gamma(\beta \to \alpha)/d\alpha$; the rate of change of P_α is then

$$\frac{dP_\alpha}{dt} = \int d\beta P_\beta \frac{d\Gamma(\beta \to \alpha)}{d\alpha} - P_\alpha \int d\beta \frac{d\Gamma(\alpha \to \beta)}{d\beta}$$

It follows immediately that $\int P_\alpha d\alpha$ is time-independent. (Just interchange the labelling of the integration variables in the integral in the second term in above Equation, On

the other hand, the rate of change of the entropy $-\int d\alpha P_x \ln P_\alpha$ is

$$-\frac{d}{dt}\int d\alpha P_z \ln P_\alpha = -\int d\alpha \int d\beta \,(\ln P_\alpha + 1) \times \left[P_\beta \frac{d\Gamma(\beta \to \alpha)}{d\alpha} - P_\alpha \frac{d\Gamma(\alpha \to \beta)}{d\beta}\right]$$

Interchanging the labelling of the integration variables in the second term, this may be written

$$-\frac{d}{dt}\int d\alpha P_\alpha \ln P_\alpha = \int d\alpha \int d\beta P_\beta \ln\left(\frac{P_\beta}{P_\alpha}\right) \frac{d\Gamma(\beta \to \alpha)}{d\alpha}.$$

Now, for any positive probabilities P_α and P_β, the function $P_\beta \ln(P_\beta/P_\alpha)$ Partial-Wave Expansions satisfies the inequality

$$P_\beta \ln\left(\frac{P_\beta}{P_\alpha}\right) \geq P_\beta - P_\alpha$$

The rate of change of the entropy is thus bounded by

$$-\frac{d}{dt}\int d\alpha P_\alpha \ln P_\alpha \geq \int d\alpha \int d\beta \,[P_\beta - P_\alpha] \frac{d\Gamma(\beta \to \alpha)}{d\alpha}$$

or interchanging variables of integration in the second term

$$-\frac{d}{dt}\int d\alpha P_\alpha \ln P_\alpha \geq \int d\alpha \int d\beta P_\beta \left[\frac{d\Gamma(\beta \to \alpha)}{d\alpha} - \frac{d\Gamma(\alpha \to \beta)}{d\beta}\right].$$

But using the unitarity relation

$$\int d\beta \frac{d\Gamma(\alpha \to \beta)}{d\beta} = \int d\beta \frac{d\Gamma(\beta \to \alpha)}{d\alpha}$$

tells us that the integral over α on the right-hand side vanishes, so we may conclude that the entropy always increases:

$$-\frac{d}{dt}\int d\alpha P_\alpha \ln P_\alpha \geq 0$$

This is the famous **Boltzman's H-theorem**

CHAPTER 3

Path Integral Formalism

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3.1 Path Integral Formulation

3.1.1 Introduction to path integral formalism in Quantum Mechanics

3.1.1.1 Action Principle and Sum over all paths

Quantum Physics and QFT can be formulated in three ways:

1)Matrix Mechanics(Heisenberg 1925)

2)Wave Mechanics(Schrödinger 1926)

3)Path Integrals(Feynman 1942-1948)

The first two versions, whose equivalence was demonstrated very early by Schrödinger, Dirac, and others, are covered in every quantum mechanics course or textbook; the third is the focus of this thesis. It was created by Feynman and is based on Dirac's work . For a long time, this formulation was thought to be excessively complex and worthless for practical reasons, thus it was left out of textbooks. The Feynman path integral, on the other hand, is easier to comprehend conceptually and needs a considerably less drastic departure from classical physics concepts (to which we are all accustomed) than the conventional quantum mechanics with its operators and state vectors in a Hilbert space. When it comes to the practical side of the various formulations, it is undeniable that Schrodinger's wave mechanics is the quickest and easiest approach to get a solution for many problems: for example, when computing the stationary states of a particle in a given potential. However, in many-particle situations, the Schrodinger equation is considerably less important, and Heisenberg's matrix mechanics is much more important (e.g. when diagonalization the Hamiltonian matrix in a certain subspace). Similarly, in field theory, the path integrals technique has become an essential tool: The Feynman rules for non-abelian gauge theories were initially obtained in this way, and numerical attempts to address the strong interaction field theory are based directly on the (Euclidean) path integral representation of Quantum Chromodynamics. Furthermore, this approach differs from other formulations in that it may be used to a wide range of physics problems. This "unification" of disparate

subjects not only aids comprehension, but also suggests new techniques that have been successful in other domains. One caveat: Except for certain circumstances (Euclidean formulation, i.e. for imaginary times Brownian motion Wiener integral), the Feynman path integral is not rigorously defined mathematically. Numerous attempts and formulations have been made to offer a mathematically solid foundation . We won't be concerned about this in our thesis because, in most situations, mathematical rigour lags well behind physical intuition. Quantum mechanics was established by Feynman in a manner similar to classical mechanics. As a result, let's start with a quick rundown of the most important parts of classical and quantum mechanics.

Classical Mechanics

A system (A point particle in one spatial dimension) with coordinate(S) q(t) is described by the Lagrangian

$$L(q(t), \dot{q}(t), t)$$

It's dynamic development, that is, its trajectory (or "path") from an initial point $q(t_a) = q_a$ to an end point $q(t_b) = q_b$ proceeds in such a way that among all possible paths the one is selected that makes the action

$$S = \int_{t_a}^{t_b} dt L(q(t), \dot{q}(t), t) \tag{3.1}$$

minimal (or more precisely:external):

$$\delta S = 0$$

From that equation of motion (Euler-Lagrangian equations) follow

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial \dot{q}} E_0 \tag{3.2}$$

and define the hamiltonian as

$$H(p(t), q(t), t) = \left[p \cdot \dot{q} - L(q, \dot{q}, t)\right]_{\dot{q}=\dot{q}(p)} \tag{3.3}$$

Hamilton's equations

$$\dot{q}(t) = \frac{\partial H}{\partial p}$$

$$\dot{p}(t) = -\frac{\partial H}{\partial q}$$

can also be obtained from an extremum of the action

$$\delta S = \delta \int_{t_a}^{t_b} dt[p \cdot \dot{q} - H(p(t), q(t), t) = 0] \tag{3.4}$$

by independent variation of q and p.

Quantum Mechanics In classical mechanics Nature seems to "compare" different paths and then to select the path of extremal action. This is also the case in optics, as long as the wavelength of light is much smaller than the typical dimensions of the system. However, if both sizes are comparable, we observe the typical interference behavior of waves, e.g. diffraction by a double slit as depicted in Fig 3.1.

The different ways now play a crucial role, since the scattered wave is composed of two parts

$$\Phi \propto= e^{ikl_1} + e^{ikl_2}$$

where k is the wave number . The intensity at the detector is proportional to $|\Phi|^2$ and shows the typical diffraction minima and maxima.

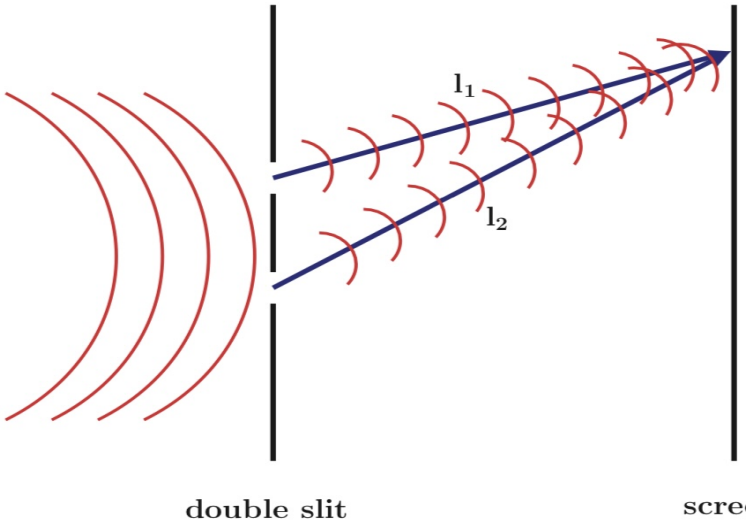

Figure 3.1: Diffraction of waves through a double slit.

It is now a crucial experimental fact that even matter particles (like electrons or neu-

trons) show diffraction effects when passing through slits or scatter from crystals. This happens when their de Broglie wavelength is comparable to the dimensions of the object to be imaged (for electrons, this was demonstrated for the first time by Davisson and Germer 1927).

The quantum mechanical description of this effect postulates a probability amplitude which is a superposition of the two possible amplitudes (for the passage through the respective slit):

$$\Phi = \Phi_1 + \Phi_2$$

and the probablity of finding the electron at the detector is ,

$$W \sim |\Phi|^2$$

in other words one has to sum coherently over the various alternative ways an event can happen.

Let us imagine that we now drill more and more holes in the screen – until it no longer exists – and that we put more and more screens in the space between source and detector which we also treat in the same way, then we have

$$\Phi(a,b) = \sum_{\text{all path from a to b}} \Phi_i$$

Of course, it remains to specify more precisely how this sum over "all paths from a to b " has to be performed and with which weight each path contributes. The answer to the first question leads to functional integrals, which we will treat in the next chapter while the problem of the weighting is solved in a heuristic way: Since Planck's constant $\hbar$ has the dimension of an action and determines the quantum effects it is not surprising that the rule is

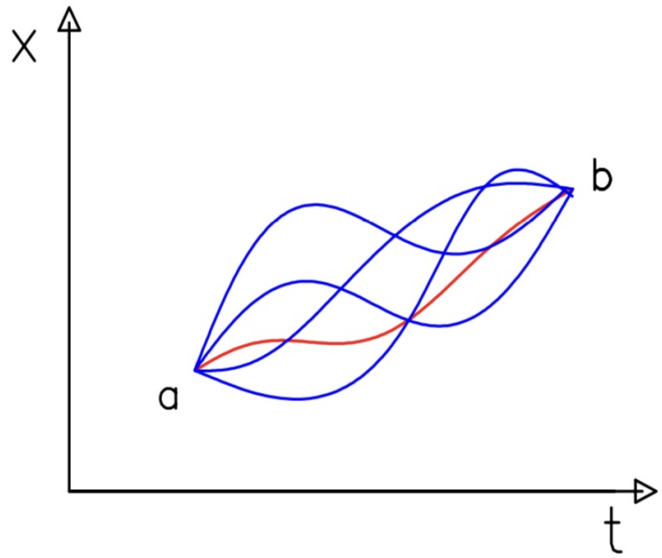

Figure 3.2: Quantum mechanical propagation of a particle from a to b. The classical path is denoted by a red line

All paths contribute with the same absolute magnitude but with different phase: The phase of every path x(t) is its classical action S[x(t)] divided by $\hbar$

$$\Phi(a,b) = \sum_{\text{all path from a to b}} const.e^{iS[x(t)]/\hbar} \tag{3.5}$$

With this prescription the classical limit (formally: $\hbar \to 0$) can be performed immediately: If all actions S>> $\hbar$ this leads to immense oscillations of the exponential function, that is, to each path with a positive contribution, there is an adjacent path which gives a negative contribution and therefore deletes it. There remains only the special path for which this doesn't happen, viz. whose phase is stationary

$$\delta S_{classical} = 0$$

and only one trajactory , contributes to the sum of all paths.

3.1.2 Path integral representation of Evolution Operator/Dynamical propagator

In the following all quantum operators are denoted by an "hat". we also assume that the Hamiltonian

$$\hat{H} = \hat{T} + \hat{V}, \hat{V} = V(x)$$

is time-independent and consider matrix elements of the time-evolution operator

$$U\left(x_b, t_b; x_a, t_a\right) = \left\langle x_b \left| \hat{U}\left(t_b, t_a\right) \right| x_a \right\rangle = \left\langle x_b \left| e^{-i(t_b - t_a)\hat{H}/\hbar} \right| x_a \right\rangle \tag{3.6}$$

As we all see, the time-evolution operator contains all information about the system that we need.

Feynmann's Path Integral

The path integral representation of U is based on the decomposition of the time interval $t_b - t_a$ into N single, infinitesimal small intervals

$$\epsilon = \frac{t_b - t_b}{N}$$

so that

$$e^{\left[-i(t_b - t_a)\hat{H}/\hbar\right]} = \lim_{N\to\infty} \prod_{k=1}^{N} e^{-i\epsilon\hat{H}/\hbar} \tag{3.7}$$

This is also called Trotter's product formula. Now it is fact that

$$e^{[-i\epsilon(\hat{T}+\hat{V})/\hbar]} = e^{[-i\epsilon\hat{T}/\hbar]} \cdot e^{[-i\epsilon\hat{V}/\hbar] + \mathcal{O}\left(\epsilon^2\right)} \tag{3.8}$$

i.e. for infinitesimal times the non-commutativity of the the quantum mechanical operators can (almost) be neglected. If we use this expression in the Trotter's formulae and insert the identity operator

$$1 = \int_{-\infty}^{+\infty} dx_j \left|x_j\right\rangle \left\langle x_j\right| \quad j = 1, 2 \ldots (N-1)$$

between each factor, it is only a small step to obtain the path integral: Since for a local

potential $V(\hat{x})|x\rangle = V(x)|x\rangle$ is valid, we obtain

$$\begin{aligned} U\left(x_b, t_b; x_a, t_a\right) = \lim_{N\to\infty} \int_{-\infty}^{+\infty} dx_1 dx_2 \ldots dx_{N-1} \left\langle x_b \left| e^{-ik\hat{T}/\hbar} \right| x_{N-1} \right\rangle e^{-i\in V(x_{N-1})/\hbar} \\ \cdot \left\langle x_{N-1} \left| e^{-i\in\hat{T}/\hbar} \right| x_{N-2} \right\rangle e^{-i\epsilon V(x_{N-2})/\hbar} \ldots \\ \cdot \left\langle x_1 \left| e^{-i\hat{E}\hat{T}/\hbar} \right| x_a \right\rangle e^{-i\epsilon V(x_a)/\hbar} \end{aligned} \tag{3.9}$$

we now need the matrix elements of $e^{(-i\epsilon\hat{T}/\hbar)}$ between position eigenstates

$$\left\langle x_{j+1} \left| e^{-i\epsilon\hat{T}/\hbar} \right| x_j \right\rangle = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dp_j e^{\left(-i\frac{\epsilon}{\hbar}\frac{p_j^2}{2m}\right)} e^{ip_j\cdot(x_{j+1}-x_j)/\hbar} \tag{3.10}$$

Here we have used that $\hat{T} = \hat{p}^2/(2m)$ is diagonal in momentum space. The integral in (3.10) is an extended Gaussian integral which can be derived from the basic integral

$$G(a) = \int_{-\infty}^{+\infty} dx e^{-ax^2} = \sqrt{\frac{\pi}{a}}, \quad \mathrm{Re}\, a > 0$$

by completion of the square:

$$\int_{-\infty}^{+\infty} dx . e^{\left(-ax^2+bx\right)} = \sqrt{\frac{\pi}{a}} . e^{\left(\frac{b^2}{4a}\right)} \quad , a \neq 0, \mathrm{Re}\, a \geq 0 \tag{3.11}$$

with this result we get

$$\left\langle x_{j+1} \left| e^{-i\epsilon\hat{T}/\hbar} \right| x_j \right\rangle = \sqrt{\frac{m}{2\pi i\epsilon\hbar}} . e^{\left[\frac{im}{2\hbar}\frac{\left(x_{j+1}-x_j\right)^2}{\epsilon}\right]} \tag{3.12}$$

and if, for notational simplification, we set

$$x_0 = x_a, x_N = x_b$$

we have

$$\begin{aligned} U\left(x_b, t_b; x_a, t_a\right) = \lim_{N\to\infty} \left(\frac{m}{2\pi i\epsilon\hbar}\right)^{N/2} \int_{-\infty}^{+\infty} dx_1 dx_2 \ldots dx_{N-1} \\ \cdot \prod_{j=0}^{N-1} e^{\left[\frac{im}{2\epsilon\hbar}(x_{j+1}-x_j)^2\right]} . e^{\left[\frac{-i\epsilon}{\hbar}V(x_j)\right]} . \end{aligned} \tag{3.13}$$

The product of exponential term is the exponent of their sum and we obtain

$$\begin{aligned} U\left(x_b,t_b;x_a,t_a\right) &= \lim_{N\to\infty}\left(\frac{m}{2\pi i\epsilon\hbar}\right)^{N/2}\int_{-\infty}^{+\infty} dx_1 dx_2\ldots dx_{N-1} \\ &\quad\cdot\exp\left\{\frac{i\epsilon}{\hbar}\sum_{j=0}^{N-1}\left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\epsilon}\right)^2 - V\left(x_j\right)\right]\right\} \\ &\equiv \int_{x(t_a)=x_a}^{x(t_b)=x_b}\mathcal{D}x(t)e^{iS[x(t)]/\hbar} \end{aligned} \tag{3.14}$$

The last line is a symbolic shorthand for the limit

$$N\to\infty,\epsilon\to 0 \qquad ;\epsilon N = t_b - t_a$$

of the (N-1)-dimensional integral. It is indeed the action which appears in the argument of the exponential function in this limit because the discrete sums approximate the Riemann integral

$$\begin{aligned} \epsilon\sum_{j=0}^{N-1}\left[\frac{m}{2}\left(\frac{\left(x_{j+1}-x_j\right.}{\epsilon}\right)^2 - V\left(x_j\right)\right] &\longrightarrow \int_{t_a}^{t_b} dt\left[\frac{m}{2}\dot{x}(t)^2 - V(x(t))\right] \\ &= \int_{t_a}^{t_b} dt L(x(t),\dot{x}(t)) = S[x(t)]. \end{aligned} \tag{3.15}$$

Note that the short -time approximation

$$\exp[-i\epsilon(\hat{T}+\hat{V})/\hbar] = \exp[-i\epsilon\hat{V}/\hbar]\cdot\exp[-i\epsilon\hat{T}/\hbar] + \mathcal{O}\left(\epsilon^2\right) \tag{3.16}$$

leads to an action in which $V(x_j+1)$ appears instead of $V(x_j)$. In a similar way the more symmetric form

$$\exp[-i\epsilon(\hat{T}+\hat{V})/\hbar] = \exp[-i\epsilon\hat{V}/(2\hbar)]\cdot\exp[-i\epsilon\hat{T}/\hbar]\cdot\exp[-i\epsilon\hat{V}/(2\hbar)] + \mathcal{O}\left(\epsilon^3\right) \tag{3.17}$$

would lead to a slightly different discrete action. In the simple case under discussion (one particle in a scalar potential) this does not lead to any consequence: The differences are of order ϵ and vanish in the continuum limit $\epsilon\to 0$. The situation is different if one considers velocity-dependent interactions because the velocity is represented by $\left(x_{j+1}-x_j\right)/\epsilon$. More on that under the heading "Ordering Problem".

The expression (3.14) gives an exact prescription how to sum over "all paths from a to b" : One discretizes the time and approximates each possible path from a to b by a polygon path. Integration over an intermediate point x_j corresponds to the summation over all paths from x_{j-1} to x_{j+1}, because with fixed x_{j-1}, x_{j+1} a new path is generated by a different value of x_j. There is no integration over the endpoints because they are fixed by the boundary conditions. An extraordinary aspect of the path integrals

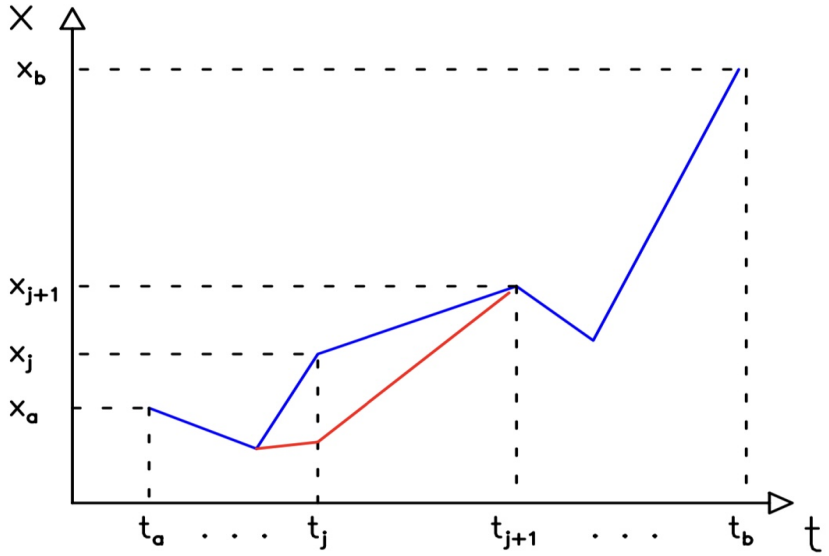

Figure 3.3: Discretization and summation over the quantum mechanical paths. The red path arises from a different value of x_j

is that they deal with ordinary numbers and not with non-commuting operators! This is an enormous advantage compared to the usual formulation of quantum mechanics. The price one has to pay for that is hidden in the complicated definition of the path integral: It is an infinite-dimensional integral, a so-called functional integral. It can be shown that the usual Schrödinger theory follows from Equation 3.14 .

Phase Space Path Integral We obtain another form of the path integral if the p -integration of the Gaussian integral is not performed:

$$\begin{aligned} U\left(x_b, t_b; x_a, t_a\right) &= \lim_{N\to\infty} \int_{-\infty}^{+\infty} dx_1 dx_2 \ldots dx_{N-1} \int_{-\infty}^{+\infty} \frac{dp_1}{2\pi\hbar}\frac{dp_2}{2\pi\hbar}\cdots\frac{dp_N}{2\pi\hbar} \\ &\quad \cdot \exp\left\{\frac{i\epsilon}{\hbar}\sum_{j=1}^{N}\left[p_j \cdot \frac{x_j - x_{j-1}}{\epsilon} - \frac{p_j^2}{2m} - V\left(x_{j-1}\right)\right]\right\} \\ &\equiv \int_{x(t_a)=x_a}^{x(t_b)=x_b} \frac{\mathcal{D}'x(t)\mathcal{D}p(t)}{2\pi\hbar} \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt[p(t)\cdot\dot{x}(t) - H(p(t),x(t))]\right\} \end{aligned} \tag{3.18}$$

Some comments about the "phase space" or Hamiltonian formulation:

1. The argument of the exponential is again the classical action divided by the action quantum, but this time formulated in coordinates and canonical momenta .

2. The "integration measure" $dx_j dp_j/(2\pi\hbar)$ is different from the Lagrangian formulation; for distinction we therefore use the notation $\mathcal{D}'x(t)$. This is descriptive and easily remembered as dividing the phase space into cells of the size $h = 2\pi\hbar$ (as in statistical mechanics).

3. There is an additional integration over dp_N and no boundary conditions for the momenta.

4. The interpretation is more difficult: Is this a sum over trajectories in phase space? Classically, however, a single point in phase space determines the trajectory.

5. While in the Lagrangian formulation the paths are continous and only the velocities are discontinuous (see Fig. 3.3), in the phase-space path integral the paths are discontinuous as well. Therefore caution is needed when performing canonical transformations and other manipulations .

6. Klauder has shown that by introducing a regularizing factor

$$\lim_{\nu\to\infty}\int \mathcal{D}x\mathcal{D}p \exp\left\{\frac{i}{\hbar}S[x,p]\right\}\cdot\exp\left[-\frac{1}{2\nu\hbar}\int_{t_a}^{t_b} dt\left(m^2\dot{x}^2 + \frac{\dot{p}^2}{m^2}\right)\right]$$

the phase space path integral can be defined unambigously.

The Ordering Problem If a classical Hamiltonian is given, in which products of coordinates and momenta occur, the question arises how to quantize such forms

"No rule based on the correspondence with Classical Mechanics can resolve such ambiguities, since the latter arise from the non-commutability of operators, which in turn is tied to the finite and non-zero character of $\hbar \ldots$ In all cases of practical interest, one must conform to the following prescriptions: ... Having put the Hamiltonian function into the form $\sum_i p_i f_i (q_1 \ldots q_n)$ one replaces... (this) term... by the symmetrized expression $\frac{1}{2} \sum_i \left[\hat{p}_i \hat{f}_i + \hat{f}_i \hat{p}_i\right]$

How do these ambiguities show up in the path integral? Obviously not in the symbolic notation as used in Eq. (1.30) and (1.46)! Actually, they appear in the innocent-looking problem how the Hamilton function is treated in the discretized form of the path integral, e.g.

a) outer averaging: $\frac{1}{2} [H (p_j, x_j) + H (p_j, x_{j-1})]$

b) inner averaging: $H \left(p_j, \frac{x_j + x_{j-1}}{2}\right)$

c) right hand: $H (p_j, x_j)$

d) left hand: $H (p_j, x_{j-1})$.

If there are no products of x and p in the Hamiltonian, then - as discussed before − the various procedures give identical results and one can chose the simplest formulation. In the general case one can show that for the treatment of products of the form

$$A := p^m x^n \tag{3.19}$$

in the Hamilton function, there exists the following correspondence between the above path integral prescriptions and the operator ordering:

a) $\frac{1}{2} [\hat{p}^m \hat{x}^n + \hat{x}^n \hat{p}^m]$

b) $\frac{1}{2^n} \sum_{k=0}^{n} \begin{pmatrix} n \\ k \end{pmatrix} \hat{x}^k \hat{p}^m \hat{x}^{n-k}$

c) $\hat{x}^n \hat{p}^m$

d) $\hat{p}^m \hat{x}^n$

Since $\hat{x}, \hat{p}$ are hermitean operators, only the symmetric forms a) and b) also give hermitean operators. Rule b) is called Weyl's quantization rule or "mid-point rule" and is obtained automatically if Eq. (3.19) is considered as Wigner transform

$$A \equiv A_W(x,p) = \int_{-\infty}^{+\infty} dy \left\langle x - \frac{y}{2} | \hat{A} | x + \frac{y}{2} \right\rangle e^{ip\cdot y/\hbar} \tag{3.20}$$

of the corresponding quantum mechanical operator $\hat{A}$. The reverse transform is

$$\left\langle x | \hat{A} | x' \right\rangle = \int_{-\infty}^{+\infty} \frac{dp}{2\pi\hbar} A_W \left(\frac{x+x'}{2}, p \right) e^{ip\cdot(x-x')/\hbar} \tag{3.21}$$

If we apply this to each factor in Trotter's product formula, we obtain

$$\begin{aligned} \left\langle x_{j+1} \left| e^{-i\epsilon\hat{H}/\hbar} \right| x_j \right\rangle &= \int_{-\infty}^{+\infty} \frac{dp_j}{2\pi\hbar} \underbrace{\left(e^{-i\epsilon\hat{H}/\hbar} \right)_W \left(\frac{x_{j+1}+x_j}{2}, p_j \right)}_{=1-i\epsilon H_W((x_{j+1}+x_j)/2, p_j)/\hbar + \ldots} e^{ip_j\cdot(x_{j+1}-x_j)/\hbar} \\ &\simeq \int_{-\infty}^{+\infty} \frac{dp_j}{2\pi\hbar} \exp\left[-\frac{i\epsilon}{\hbar} H_W \left(\frac{x_{j+1}+x_j}{2}, p_j \right) \right] e^{ip_j\cdot(x_{j+1}-x_j)/\hbar} \end{aligned} \tag{3.22}$$

which leads to a generalization of Eq. (1.45) for arbitrary Hamilton functions and which contains the mid-point rule. The ordering prescription becomes important for curvi-linear coordinates or for quantization in curved spaces. A less exotic application is the case of a charged particle in a magnetic field because the minimal substitution for the electromagnetic field leads to the velocity-dependent Lorentz force.

3.1.3 Perturbation Theory and Retrieval of Interaction Picture Time Evolution Operator

We now consider the (for simplicity again: one-dimensional) motion of a particle in a general potential $V(x)$, i.e. Lagrange functions of the form

$$L = \frac{m}{2}\dot{x}^2 - V(x)$$

In general the path integral cannot be evaluated anymore,A widely used method for weak interactions (potentials) is perturbation theory, which we may obtain from the

phase space formula (3.18) by expansion in powers of the potential:

$$\begin{aligned} U\left(x',t';x,t\right) &= \int_{x(t)=x}^{x(t')=x'} \frac{\mathcal{D}'x\mathcal{D}_p}{2\pi\hbar} \exp\left[\frac{i}{\hbar}\int_t^{t'} d\sigma\left(p\dot{x}-\frac{p^2}{2m}\right)\right] \sum_{j=0}^{\infty}\left(-\frac{i}{\hbar}\right)^j \frac{1}{j!}\left(\int_t^{t'} d\tau V(x(\tau))\right)^j \\ &=: \sum_{j=0}^{\infty}\left(-\frac{i}{\hbar}\right)^j U_j\left(x',t';x,t\right) \end{aligned} \tag{3.23}$$

The first term is the free propagator which is given by

$$\begin{aligned} U_0\left(x_b,t_b;x_a,t_a\right) &= \int_{-\infty}^{+\infty} \frac{dp}{2\pi\hbar} \exp\left[\frac{i}{\hbar}\left(p\cdot\left(x_b-x_a\right)-\frac{p^2}{2m}T\right)\right] \\ &= \sqrt{\frac{m}{2\pi i\hbar T}} \exp\left[\frac{im}{2\hbar T}\left(x_b-x_a\right)^2\right] \end{aligned} \tag{3.24}$$

Put $x_b = x^{'}$, $x_a = x$ and $t^{'} - t = T$

$$U_0\left(x',t';x,t\right) = \int_{-\infty}^{+\infty} \frac{dp}{2\pi\hbar} \exp\left\{\frac{i}{\hbar}\left[p\left(x'-x\right)-\frac{p^2}{2m}\left(t'-t\right)\right]\right\}. \tag{3.25}$$

Let us now consider the next term of the perturbation expansion 3.23

$$U_1\left(x',t';x,t\right) = \int_{x(t)=x}^{x(t')=x'} \frac{\mathcal{D}'x\mathcal{D}_p}{2\pi\hbar} \exp\left[\frac{i}{\hbar}\int_t^{t'} d\sigma\left(p\dot{x}-\frac{p^2}{2m}\right)\right] \int_t^{t'} d\tau V(x(\tau))$$

In the discretized form the last factor is

$$\int_t^{t'} d\tau V(x(\tau)) = \epsilon\sum_{j=1}^{N} V\left(x_j\right), \qquad \text{with } \epsilon = \frac{t'-t}{N}$$

and thus

$$U_1(x',t';x,t) = \lim_{N\to\infty} \epsilon \sum_{j=1}^{N} \prod_{k=1}^{N-1} \left(\int_{-\infty}^{+\infty} \frac{dx_k dp_k}{2\pi\hbar} \right) \int_{-\infty}^{+\infty} \frac{dp_N}{2\pi\hbar} V(x_j) \\ \times \exp\left\{ \frac{i}{\hbar} \sum_{l=1}^{N} \left[p_l (x_l - x_{l-1}) - \epsilon \frac{p_l^2}{2m} \right] \right\} \tag{3.26}$$

Similarly as in the evaluation of the free propagator we write the exponent as

$$\frac{i}{\hbar} \left[\sum_{l=1}^{N-1} (p_l - p_{l+1}) x_l + p_N x' - p_1 x - \epsilon \sum_{l=1}^{N} \frac{p_l^2}{2m} \right]$$

and perform all x_k -integrations (except x_j). This gives $(N-2)$ momentum δ -functions

$$U_1(x',t';x,t) = \lim_{N\to\infty} \epsilon \sum_{j=1}^{N} \int_{-\infty}^{+\infty} dx_j V(x_j) \prod_{k=1}^{N} \left(\int_{-\infty}^{+\infty} \frac{dp_k}{2\pi\hbar} \right) (2\pi\hbar)^{N-2} \\ \cdot \delta(p_1 - p_2)\, \delta(p_2 - p_3) \ldots \delta(p_{j-1} - p_j)\, \delta(p_{j+1} - p_{j+2}) \ldots \delta(p_{N-1} - p_N) \\ \cdot \exp\left\{ \frac{i}{\hbar} \left[(p_j - p_{j+1}) x_j + p_N x' - p_1 x \right] - \epsilon \sum_{l=1}^{N} \frac{p_l^2}{2m} \right\}$$

These enforce $p_1 = p_2 = \ldots p_{j-1} = p_j$ and $p_{j+1} = p_{j+2} = \ldots p_{N-1} = p_N$, so that we obtain

$$U_1(x',t';x,t) = \lim_{N\to\infty} \epsilon \sum_{j=1}^{N} \int_{-\infty}^{+\infty} dx_j V(x_j) \int_{-\infty}^{+\infty} \frac{dp_j dp_N}{(2\pi\hbar)^2} \exp\left\{ \frac{i}{\hbar} \left[(p_j - p_N) x_j + p_N x' - p_j x \right] \right\} \cdot \tag{3.27}$$

$$\exp\left[-\frac{i}{\hbar} \epsilon \left(\frac{p_j^2}{2m} j + \frac{p_N^2}{2m} (N - j) \right) \right] \tag{3.28}$$

If we now write $\xi = x_j, p = p_j$ and $p' = p_N$, the result is

$$U_1(x',t';x,t) = \lim_{N\to\infty} \epsilon \sum_{j=1}^{N} \int_{-\infty}^{+\infty} d\xi V(\xi) \underbrace{\int_{-\infty}^{+\infty} \frac{dp'}{2\pi\hbar} \exp\left\{\frac{i}{\hbar}\left[(x'-\xi)\,p' - \frac{p'^2}{2m}\epsilon(N-j)\right]\right\}}_{=U_0(x',t';\xi,t+j\epsilon)} \underbrace{\int_{-\infty}^{+\infty} \frac{dp}{2\pi\hbar} \exp\left\{\frac{i}{\hbar}\left[(\xi-x)p - \frac{p^2}{2m}j\epsilon\right]\right\}}_{=U_0(\xi,t+j\epsilon;x,t)}. \tag{3.29}$$

It is now possible to perform the limit which gives a Riemannian integral over the intermediate time $\tau, (\tau_j = t + j\epsilon)$

$$U_1(x',t';x,t) = \int_t^{t'} d\tau \int_{-\infty}^{+\infty} d\xi U_0(x',t';\xi,\tau)\, V(\xi) U_0(\xi,\tau;x,t) \tag{3.30}$$

Read from right to left this contribution to the perturbative expansion can be depicted as a Feynman diagram as shown below

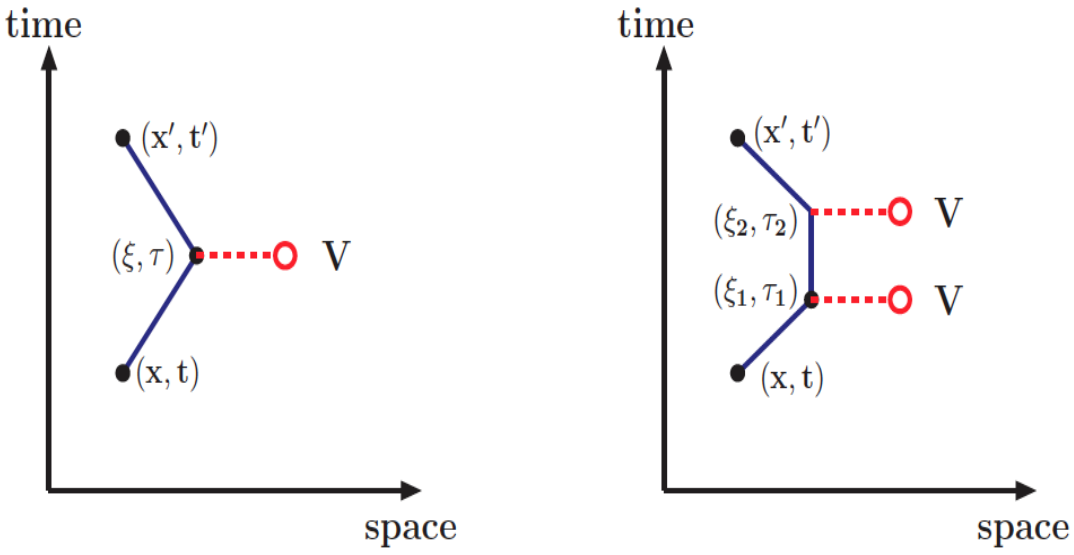

Figure 3.4: (a) Feynman diagram in 1st order perturbation theory for the time-evolution operator in Eq.(3.30).The solid blue lines represent the free propagator between two space-time points, the dashed red line the interaction of the potential V . Intermediate points are to be integrated over. (b) Feynman diagram for the 2nd order, see Eq. (3.32)

Similarly one proceeds in higher orders

$$U_j\left(x',t';x,t\right)=\frac{1}{j!}\int_{x(t)=x}^{x(t')=x'}\frac{\mathcal{D}'x\mathcal{D}p}{2\pi\hbar}\exp\left[\frac{i}{\hbar}\int_t^{t'}d\sigma\left(p\dot{x}-\frac{p^2}{2m}\right)\right]\left(\int_t^{t'}d\tau V(x(\tau))\right)^j$$

By induction one can prove that

$$\left(\int_t^{t'}d\tau V(x(\tau))\right)^j=j!\int_t^{t'}d\tau_1\int_t^{\tau_1}d\tau_2\ldots\int_t^{\tau_{j-1}}d\tau_j V\left(x\left(\tau_1\right)\right)V\left(x\left(\tau_2\right)\right)\ldots V\left(x\left(\tau_j\right)\right)$$

which - with a similar calculation - leads to

$$U_j\left(x',t';x,t\right)=\int_t^{t'}d\tau\int_{-\infty}^{+\infty}d\xi U_0\left(x',t';\xi,\tau\right)V(\xi)U_{j-1}(\xi,\tau;x,t),j=1,2,\ldots \quad (3.31)$$

The graphical representation for $j=2$

$$\begin{aligned}U_2\left(x',t';x,t\right)=&\int_t^{t'}d\tau_2\int_{-\infty}^{+\infty}d\xi_2 U_0\left(x',t';\xi_2,\tau_2\right)V\left(\xi_2\right)\\&\int_t^{\tau_2}d\tau_1\int_{-\infty}^{+\infty}d\xi_1 U_0\left(\xi_2,\tau_2;\xi_1,\tau_1\right)V\left(\xi_1\right)U_0\left(\xi_1,\tau_1;x,t\right)\end{aligned} \quad (3.32)$$

is shown in Fig. 3.4b . Insertion of the recursion relation (3.31) into Eq. (3.23) gives an integral equation for the time-evolution operator

$$U\left(x',t';x,t\right)=U_0\left(x',t';x,t\right)-\frac{i}{\hbar}\int_t^{t'}d\tau\int_{-\infty}^{+\infty}d\xi U_0\left(x',t';\xi,\tau\right)V(\xi)U(\xi,\tau;x,t) \quad (3.33)$$

This is the usual equation for the time-evolution operator in the **interaction picture** as one can see if one writes above Equation in the operator form

$$\hat{U}\left(t',t\right)=\hat{U}_0\left(t',t\right)-\frac{i}{\hbar}\int_t^{t'}d\tau\hat{U}_0\left(t',\tau\right)\hat{V}\hat{U}(\tau,t) \quad (3.34)$$

Defining

$$\hat{U}\left(t',t\right)=:\hat{U}_0\left(t',t\right)\hat{U}_I\left(t',t\right)$$

one obtains

$$\hat{U}_0(t',t)\,\hat{U}_I(t',t) = \hat{U}_0(t',t) - \frac{i}{\hbar}\int_t^{t'} d\tau \underbrace{\hat{U}_0(t',\tau)}_{=\hat{U}_0(t',t)\hat{U}_0(t,\tau)=\hat{U}_0(t',t)\hat{U}_0^\dagger(\tau,t)} \hat{V}\hat{U}(\tau,t) \qquad (3.35)$$

Here the composition law for the free propagator $\hat{U}_0$ has been used. Multiplying from the left with $\hat{U}_0^{-1}(t',t)$ one obtains

$$\hat{U}_I(t',t) = 1 - \frac{i}{\hbar}\int_t^{t'} d\tau \underbrace{\hat{U}_0^\dagger(\tau,t)\hat{V}\hat{U}_0(\tau,t)}_{=:V_I(t',t)}\hat{U}_I(\tau,t),$$

which is identical with the equation of motion for the time-evolution operators in the interaction picture. From the derivation of Eq. (3.33) it is clear that this equation is also valid for time-dependent potentials. However, if the potential is time-independent then the integral term on the right side of Eq.(3.34) is a convolution integral, since the evolution operators then only depend on the time difference. According to well known theorems for the Fourier transformation we then immediately obtain for the time-independent Green function

$$\hat{G}(E) = \int_{-\infty}^{+\infty} dt\hat{G}(t)e^{iEt/\hbar}, \text{ with } \hat{G}(t) := -\frac{i}{\hbar}\Theta(t)\hat{U}(t,0) \qquad (3.36)$$

According to the Lippmann-Schwinger equation

$$\hat{G}(E) = \hat{G}_0(E) + \hat{G}_0(E)\hat{V}\hat{G}(E),$$

which simply is the operator identity

$$\frac{1}{E-\hat{H}+i0^+} = \frac{1}{E-\hat{H}_0+i0^+} + \frac{1}{E-\hat{H}_0+i0^+}\hat{V}\frac{1}{E-\hat{H}+i0^+}.$$

The prescription that the singularity in these operators has to be regularized by adding $+i\times$ an infinitesimal positive quantity in the denominator follows from the definition (3.36) in which the energy E must have a small, positive imaginary part in order that the time integral converges.

3.1.4 Greens Function as Path Integrals and Time ordering in Path Integrals

Up to now we have discussed the path-integral representation of the time-evolution operators $\hat{U}$ in different formulations. Now we want to consider 2-point Green functions of the form

$$G_{AB}\left(t_1, t_2\right) := \left\langle 0 \left| \mathcal{T}\left[\hat{A}_H\left(t_1\right)\hat{B}_H\left(t_2\right)\right] \right| 0 \right\rangle \tag{3.37}$$

where $\mid 0\rangle$ is the exact ground state of the system,

$$\hat{A}_H(t) = e^{i\hat{H}t/\hbar}\hat{A}_H(0)e^{-i\hat{H}t/\hbar}$$

is a quantum mechanical operator in the Heisenberg picture (as is $\hat{B}_H(t)$) and

$$\mathcal{T}\left[\hat{A}_H\left(t_1\right)\hat{B}_H\left(t_2\right)\right] = \Theta\left(t_1 - t_2\right)\hat{A}_H\left(t_1\right)\hat{B}_H\left(t_2\right) + \Theta\left(t_2 - t_1\right)\hat{B}_H\left(t_2\right)\hat{A}_H\left(t_1\right)$$

the time-ordered product of these two operators. Such objects play a central role in many-body physics and in field theory, as it is straight-forward to evaluate them in perturbation theory and all important quantities (ground-state energy, expectation values of operators, S matrix elements) can be calculated from them. If we insert into the definition (3.37) a complete set of position eigenstates

$$1 = \int dq|q\rangle\langle q| = \int dq.e^{i\hat{H}t/\hbar}|q\rangle\langle q|e^{-i\hat{H}t/\hbar},$$

then we obtain

$$\begin{aligned} G_{AB}\left(t_1, t_2\right) = \int dqdq' \left\langle 0 \left| e^{i\hat{H}t'/\hbar} \right| q' \right\rangle \left\langle q' \left| e^{-i\hat{H}t'/\hbar} \mathcal{T}\left[\hat{A}_H\left(t_1\right)\hat{B}_H\left(t_2\right)\right] e^{i\hat{H}t/\hbar} \right| q \right\rangle \\ \cdot \left\langle q \left| e^{-i\hat{H}t/\hbar} \right| 0 \right\rangle \end{aligned} \tag{3.38}$$

The individual factors in this expression may be rewritten in the following way: The first one

$$\left\langle 0 \left| e^{i\hat{H}t'/\hbar} \right| q' \right\rangle = e^{iE_0t'/\hbar}\langle 0\,|q'\rangle = e^{iE_0t'/\hbar}\psi_0^\star\left(q'\right)$$

can be expressed by the wave function of the ground state and the ground-state energy - similarly, also the last one.Therefore we now concentrate on a path-integral represen-

tation for the middle factor and first assume that $\hat{A} = \hat{B} = \hat{x}$ and that $t_1 > t_2$. After inserting two complete sets of position eigenstates we then obtain

$$\left\langle q' \left| e^{-i\hat{H}t'/\hbar} \hat{x}_H(t_1)\, \hat{x}_H(t_2)\, e^{i\hat{H}t/\hbar} \right| q \right\rangle = \left\langle q' \left| e^{-i\hat{H}(t'-t_1)/\hbar} \hat{x} e^{-i\hat{H}(t_1-t_2)/\hbar} \hat{x} e^{-i\hat{H}(t_2-t)} \right| q \right\rangle$$
$$= \int dq_1 dq_2 q_1 q_2 \left\langle q' \left| e^{-i\hat{H}(t'-t_1)/\hbar} \right| q_1 \right\rangle \left\langle q_1 \left| e^{-i\hat{H}(t_1-t_2)/\hbar} \right| q_2 \right\rangle \left\langle q_2 \left| e^{-i\hat{H}(t_2-t)/\hbar} \right| q \right\rangle$$

Now we may use the path-integral representation of the individual time-evolution operators and obtain in the Hamilton formulation

$$\begin{aligned}
&\left\langle q' \left| e^{-i\hat{H}t'/\hbar} \hat{x}_H(t_1)\, \hat{x}_H(t_2)\, e^{i\hat{H}t/\hbar} \right| q \right\rangle \\
&= \int dq_1 dq_2 q_1 q_2 \int_{x(t_1)=q_1}^{x(t')=q'} \frac{\mathcal{D}'x\mathcal{D}p}{2\pi\hbar} \exp\left\{ \frac{i}{\hbar} \int_{t_1}^{t'} d\tau [p\dot{x} - H(x,p)] \right\} \\
&\cdot \int_{x(t_2)=q_2}^{x(t_1)=q_1} \frac{\mathcal{D}'x\mathcal{D}p}{2\pi\hbar} \exp\left\{ \frac{i}{\hbar} \int_{t_2}^{t_1} d\tau [p\dot{x} - H(x,p)] \right\} \\
&\cdot \int_{x(t)=q}^{x(t_2)=q_2} \frac{\mathcal{D}'x\mathcal{D}p}{2\pi\hbar} \exp\left\{ \frac{i}{\hbar} \int_{t}^{t_2} d\tau [p\dot{x} - H(x,p)] \right\}
\end{aligned}$$

Now we can concentrate the exponents into one exponent and all integrations can be combined into one functional integral if one integrates additionally over the endpoints q_1, q_2. For $t_1 > t_2$ the result therefore is

$$\begin{aligned}
&\langle q'|\, e^{-i\hat{H}t'/\hbar} \mathcal{T}\left[\hat{x}_H(t_1)\, \hat{x}_H(t_2)\right] e^{i\hat{H}t/\hbar} |q\rangle \\
&\qquad = \int_{x(t)=q}^{x(t')=q'} \frac{\mathcal{D}'x\mathcal{D}p}{2\pi\hbar} x(t_1)\, x(t_2) \exp\left\{ \frac{i}{\hbar} \int_{t}^{t'} d\tau [p\dot{x} - H(x,p)] \right\}
\end{aligned} \tag{3.39}$$

For $t_2 > t_1$, a similar calculation gives the same expression, i.e. **the time-ordering operator is automatically built into the path-integral representation!** This is not quite so surprising as it first seems, since the time ordering is necessary because the Heisenberg operator do not commute at different times − the path integral, however, deals with ordinary numbers.

Eq. (3.39) is easily generalized to any operator $\hat{A} = A(\hat{x}, \hat{p}), \hat{B} = B(\hat{x}, \hat{p})$ and then it

becomes

$$\begin{aligned}&\left\langle q'\left|e^{-i\hat{H}t'/\hbar}\mathcal{T}\left[\hat{A}_H\left(t_1\right)\hat{B}_H\left(t_2\right)\right]e^{i\hat{H}t/\hbar}\right|q\right\rangle \\ &=\int_{x(t)=q}^{x(t')=q'}\frac{\mathcal{D}'x\mathcal{D}p}{2\pi\hbar}A\left(p\left(t_1\right),x\left(t_1\right)\right)B\left(p\left(t_2\right),x\left(t_2\right)\right)\exp\left\{\frac{i}{\hbar}S[x(t),p(t)]\right\}\end{aligned} \tag{3.40}$$

Let us return to the formula (3.38) for the Green function in which we now can insert the above result. However, the appearance of the ground-state wave function $\psi_0(q)$ is unsatisfactory since the exact ground state is unknown in general. We would like to have an expression available in which the ground state is generated at the same time. This is possible by "filtering" out the lowest lying state of the system. Indeed, in an expression of the form

$$\left\langle q'\left|e^{-i\hat{H}t'/\hbar}\hat{\mathcal{O}}e^{i\hat{H}t/\hbar}\right|q\right\rangle=\sum_{n,m}\psi_m\left(q'\right)e^{-iE_mt'/\hbar}\langle m|\hat{\mathcal{O}}|n\rangle e^{iE_nt/\hbar}\psi_n^\star(q)$$

only the ground state contribution survives if one formally approach by doing a **Wick rotation** and get it in the form of a **Eucledian Path Integral**

$$t\to i\infty,\quad t'\to-i\infty$$

and get

$$\begin{aligned}\left\langle q'\left|e^{-i\hat{H}t'/\hbar}\hat{\mathcal{O}}e^{i\hat{H}t/\hbar}\right|q\right\rangle &\overset{t\to i\infty}{\longrightarrow}\overset{t'\to-i\infty}{\longrightarrow}\psi_0\left(q'\right)\psi_0^\star(q)e^{-E_0(|t|+|t'|)/\hbar}\langle0|\hat{\mathcal{O}}|0\rangle \\ &=\lim_{\substack{t\to i\infty\\t'\to-i\infty}}\left\langle q'\left|e^{-i\hat{H}(t'-t)/\hbar}\right|q\right\rangle\langle0|\hat{\mathcal{O}}|0\rangle.\end{aligned} \tag{3.41}$$

This is due to the fact that for $n>0, E_n>E_0$, so that the contributions of the excited states decay more rapidly than those from the ground state. If we use above Eq. (3.41) for the Green function of the operators $\hat{A},\hat{B}$ we obtain

$$G_{AB}\left(t_1,t_2\right)=\lim_{\substack{t\to i\infty\\t'\to-i\infty}}\frac{\left\langle q'\left|e^{-i\hat{H}t'/\hbar}\mathcal{T}\left[\hat{A}_H\left(t_1\right)\hat{B}_H\left(t_2\right)\right]e^{i\hat{H}t/\hbar}\right|q\right\rangle}{\left\langle q'\left|e^{-i\hat{H}(t'-t)/\hbar}\right|q\right\rangle} \tag{3.42}$$

or as path integral form

$$G_{AB}\left(t_1,t_2\right)=\lim_{\substack{t\to i\infty\\t'\to-i\infty}}\frac{\int\mathcal{D}'x\mathcal{D}pA\left(x\left(t_1\right),p\left(t_1\right)\right)B\left(x\left(t_2\right),p\left(t_2\right)\right)e^{iS[x,p]/\hbar}}{\int\mathcal{D}'x\mathcal{D}pe^{iS[x,p]/\hbar}} \tag{3.43}$$

Note that in the expression (3.43) all normalization factors cancel! The unphysical limits $t \to i\infty, \quad t' \to -i\infty$ are quite natural for Euclidean Green functions where the time t is replaced by $-i\tau$ everywhere. Instead of oscillations one has damping everywhere and the path integral ist well-defined mathematically. Therefore one frequently investigates Euclidean Green functions and transforms back - if possible - to real time by an analytic continuation. It is clear that in order to project out the ground state by the boundary conditions $t \to i\infty, \quad t' \to -i\infty$ one doesn't necessarily have to go to infinity along the imaginary axis but that it is sufficient to do that along a suitable ray in the complex time plane

The operators $\hat{A}, \hat{B}$ can be expressed in terms of the fundamental operators $\hat{x}, \hat{p}$, say by a Taylor expansion. However, it is not necessary that in the matrix element the products of operators $\hat{x}, \hat{p}$ all are taken at the same time: One can define **n-point correlation functions** in quantum mechanics as

$$G\left(t_1 \ldots t_j, t_{j+1} \ldots t_n\right) := \left\langle 0 \left| \mathcal{T}\left[\hat{x}_H\left(t_1\right) \ldots \hat{x}_H\left(t_j\right) \hat{p}_H\left(t_{j+1}\right) \ldots \hat{p}_H\left(t_n\right)\right] \right| 0 \right\rangle \tag{3.44}$$

which takes the form

$$G\left(t_1 \ldots t_j, t_{j+1} \ldots t_n\right) = \frac{\int \mathcal{D}' x \mathcal{D} p x\left(t_1\right) \ldots x\left(t_j\right) p\left(t_{j+1}\right) \ldots p\left(t_n\right) e^{iS[x,p]/\hbar}}{\int \mathcal{D}' x \mathcal{D} p e^{iS[x,p]/\hbar}}. \tag{3.45}$$

in the Path Integral Formulation.

The full set of n -point functions can be obtained from a **generating functional**

$$Z[J,K] = \int \mathcal{D}' x \mathcal{D} p \exp\left\{\frac{i}{\hbar} S[x,p] + \frac{i}{\hbar} \int dt [J(t)x(t) + K(t)p(t)]\right\} \tag{3.46}$$

by functional differentiation with respect to artificially introduced sources which are set to zero thereafter

$$G\left(t_1 \ldots t_j, t_{j+1} \ldots t_n\right) = (-i\hbar)^n \frac{\delta^j}{\delta J\left(t_1\right) \ldots \delta J\left(t_j\right)} \frac{\delta^{n-j}}{\delta K\left(t_{j+1}\right) \ldots \delta K\left(t_n\right)} \frac{Z[J,K]}{Z[0,0]}\Bigg|_{J=K=0} \tag{3.47}$$

.

In general the generating functional cannot be evaluated exactly. However, if one can split up the Hamiltonian

$$\hat{H} = \hat{H}_0 + V(\hat{x}, \hat{p})$$

in such a way that the generating functional $Z_0[J, K]$ is known then one can give a closed expression for the full generating functional: First one also splits up the exponent in the path integral as

$$\int dt \left[p\dot{x} - H_0(x,p) + J(t)x(t) + K(t)p(t)\right] - \int dt V(x(t), p(t))$$

and then one uses the fact that $x(t)$ can be generated by functional differentiation w.r.t. the source $J(t), p(t)$ by differentiation w.r.t. $K(t)$. With this procedure the exponent of the "perturbation" V can be taken out from the path integral and we obtain the representation

$$\begin{aligned} Z[J,K] &= \int \mathcal{D}'x\mathcal{D}p \exp\left[-\frac{i}{\hbar}\int dt V(x(t),p(t))\right] \exp\left\{\frac{i}{\hbar}S_0 + \frac{i}{\hbar}\int dt[J(t)x(t) + K(t)p(t)]\right\} \\ &= \exp\left[-\frac{i}{\hbar}\int dt V\left(\frac{\hbar}{i}\frac{\delta}{\delta J(t)}, \frac{\hbar}{i}\frac{\delta}{\delta K(t)}\right)\right] Z_0[J,K] \end{aligned} \tag{3.48}$$

Of course, this is only a formal solution and in most cases one has to expand the exponential function in powers of the perturbation in order to perform the functional differentiations. This produces the perturbation series for the generating functional and therefore for alle n -point functions.We will discuss this in detain in the next sections in Field Theory Path integrals.

3.2 Field theoretic treatment of Path Integrals

3.2.1 Functional Calculus

3.2.1.1 What are Functionals?

Mathematically Given a manifold $\mathscr{M}$ representing (continuous/smooth) functions f (with certain boundary conditions etc.), and a functional F defined as a map

$$F : \mathscr{M} \to \Re \quad \text{or} \quad F : \mathscr{M} \to \mathcal{C}, \tag{3.49}$$

It is evident that in dealing with dynamical systems, we are dealing with functions of continuous variables. In fact, most of the times, we are really dealing with functions of functions which are otherwise known as functionals. If we are considering the motion of a particle in a potential in one dimension, then the Lagrangian is given by

$$L(x, \dot{x}) = \frac{1}{2} m\dot{x}^2 - V(x)$$

where $x(t)$ and $\dot{x}(t)$ denote the coordinate and the velocity of the particle and the simplest functional we can think of is the action functional defined as

$$S[x] = \int_{t_i}^{t_f} \mathrm{d}t L(x, \dot{x}).$$

Note that unlike a function whose value depends on a particular point in the coordinate space, the value of the action depends on the entire trajectory along which the integration is carried out. For different paths connecting the initial and the final points, the value of the action functional will be different. Thus, a functional has the generic form

$$F[f] = \int \mathrm{d}x F(f(x))$$

where, for example, we may have

$$F(f(x)) = (f(x))^n.$$

Sometimes, one loosely also says that $F(f(x))$ is a functional.

3.2.1.2 Functional derivatives

The functional Derivative or the Gateaux derivative of a functional F (linear functional) is defined as

$$F'[v] = \frac{\mathrm{d}}{\mathrm{d}\epsilon} F[f + \epsilon v]\Big|_{\epsilon=0} = \int \mathrm{d}x \frac{\delta F[f]}{\delta f(x)} v(x) \tag{3.50}$$

where ν is an arbitrary function and $\epsilon\nu$ is defined as variation of f Equivalently, from the working point of view, this simply corresponds to defining

$$\frac{\delta F(f(x))}{\delta f(y)} = \lim_{\epsilon \to 0} \frac{F(f(x) + \epsilon\delta(x-y)) - F(f(x))}{\epsilon}$$

It now follows from above equation that

$$\frac{\delta f(x)}{\delta f(y)} = \delta(x-y)$$

The functional derivative satisfies all the properties of a derivative, namely, it is linear and associative,

$$\begin{aligned} \frac{\delta}{\delta f(x)} \left(F_1[f] + F_2[f]\right) &= \frac{\delta F_1[f]}{\delta f(x)} + \frac{\delta F_2[f]}{\delta f(x)} \\ \frac{\delta}{\delta f(x)} \left(F_1[f] F_2[f]\right) &= \frac{\delta F_1[f]}{\delta f(x)} F_2[f] + F_1[f] \frac{\delta F_2[f]}{\delta f(x)} \end{aligned} \tag{3.51}$$

It also satisfies the chain rule of differentiation. Furthermore, we now see that given a functional $F[f]$, we can Taylor expand it in the form

$$\begin{aligned} F[f] = &\int \mathrm{d}x P_0(x) + \int \mathrm{d}x_1 \, \mathrm{d}x_2 P_1(x_1, x_2) f(x_2) \\ &+ \int \mathrm{d}x_1 \, \mathrm{d}x_2 \, \mathrm{d}x_3 P_2(x_1, x_2, x_3) f(x_2) f(x_3) + \cdots \end{aligned}$$

where

$$\begin{aligned} P_0(x) &= F(f(x))|_{f(x)=0} \\ P_1(x_1, x_2) &= \frac{\delta F(f(x_1))}{\delta f(x_2)}\Big|_{f(x)=0} \\ P_2(x_1, x_2, x_3) &= \frac{1}{2!} \frac{\delta^2 F(f(x_1))}{\delta f(x_2) \delta f(x_3)}\Big|_{f(x)=0} \end{aligned}$$

and so on.

Functional differential: The differential (or variation or first variation) of the functional $\boldsymbol{F}[f]$ is

$$\delta F[f;\nu] = \int \frac{\delta F}{\delta f}(x)\nu(x)dx$$

Heuristically, ν is the change in f, so we 'formally' have $\nu = \delta f$, and then this is similar in form to the total differential of a function $F(f_1, f_2, \ldots, f_n)$,

$$dF = \sum_{i=1}^{n} \frac{\partial F}{\partial f_i} df_i$$

where $f_1, f_2, \ldots, f_n$ are independent variables. Comparing the last two equations, the functional derivative $\delta F/\delta f(x)$ has a role similar to that of the partial derivative $\partial F/\partial_i$, where the variable of integration x is like a continuous version of the summation index $\boldsymbol{i}$.

3.2.1.3 Functional Integration

Whereas standard Riemann integration sums a function $f(x)$ over a continuous range of values of x, functional integration sums a functional $G[f]$, which can be thought of as a "function of a function" over a continuous range (or space) of functions f. Most functional integrals cannot be evaluated exactly but must be evaluated using perturbation methods. The formal definition of a functional integral is

$$\int G[f][Df] \equiv \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} G[f] \prod_x df(x)$$

However, in most cases the functions $f(x)$ can be written in terms of an infinite series of orthogonal functions such as $f(x) = f_n H_n(x)$, and then the definition becomes

$$\int G[f][Df] \equiv \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} G(f_1, f_2, \ldots) \prod_n df_n$$

which is slightly more understandable. The integral is shown to be a functional integral with a capital D. Sometimes it is written in square brackets: $[Df]$ or $D[f]$, to indicate that f is a function.

Examples: Most functional integrals are actually infinite, but then the limit of the quotient of two related functional integrals can still be finite. The functional integrals that can be evaluated exactly usually start with the following Gaussian integral:

$$\frac{\int e^{i\int -\frac{1}{2}f(x)\cdot K(x,y)\cdot f(y)dxdy+\int J(x)\cdot f(x)dx}[Df]}{\int e^{i\int -\frac{1}{2}f(x)\cdot K(x,y)\cdot f(y)dxdy}[Df]} = e^{i\frac{1}{2}\int J(x)\cdot K^{-1}(x,y)\cdot J(y)dxdy}$$

By functionally differentiating this with respect to $J(x)$ and then setting to o this becomes an exponential multiplied by a polynomial in f. For example, setting $\boldsymbol{K}(x,\boldsymbol{y}) = \delta(\boldsymbol{x}-\boldsymbol{y})$, we find:

$$\frac{\int f(a)f(b)e^{i\int f(x)f(x)dx^4}[Df]}{\int e^{i\int f(x)f(x)dx^4[Df]}} = K^{-1}(a,b) = \frac{1}{|a-b|^2}$$

where a, b and x are 4-dimensional vectors. This comes from the formula for the propagation of a photon in quantum electrodynamics. Another useful integral is the functional delta function:

$$\int e^{i\int f(x)g(x)dx}[Df] = \delta[g] = \prod_x \delta(g(x)) \tag{3.52}$$

which is useful to specify constraints. Functional integrals can also be done over Grassmann-valued functions $\psi(x)$, where $\psi(x)\psi(y) = -\psi(y)\psi(x)$, which is useful in quantum electrodynamics for calculations involving fermions. **It is worth noting that Functional Integrals and Path integrals are same thing and only differs in the terminology used by Mathematicians(Functional Integrals) and Physicists(Path integrals).**

3.2.2 Path Integral formulation of Correlation Functions(Field theory)

3.2.2.1 PI formulation of the two-point correlation function

A further step toward a more convenient formulation of QFT is obtained by getting rid of the boundary conditions. What we are really interested in, is the set of time-ordered correlation functions among fields at different space-time points, evaluated on the ground state of the system (also know as Green's functions). Indeed, we will see how , starting from these correlation functions the LSZ reduction formulae allow us to extract the probability amplitudes for physical scattering processes, i.e. the elements of the S matrix.The simplest of such correlations is the two-point function

$$\left\langle \Omega \left| T\left\{ \hat{\phi}_H\left(x_1\right) \hat{\phi}_H\left(x_2\right) \right\} \right| \Omega \right\rangle \tag{3.53}$$

where $|\Omega\rangle$ denotes the ground state (of the interacting theory) and $\hat{\phi}_H$ the operators associated to the fields in the Heisenberg's picture.

In order to find a PI formulation of (3.53), consider the following functional integral, with generic boundary conditions at $t = \pm T$

$$I_{12} = \int \mathcal{D}\phi(x) \phi\left(x_1\right) \phi\left(x_2\right) e^{i \int_{-T}^{+T} d^4x \mathcal{L}(\phi)} \tag{3.54}$$

The main functional integral $\int \mathcal{D}\phi(x)$ can be broken up as

$$\int \mathcal{D}\phi(x) \equiv \int \mathcal{D}\phi_1(\vec{x}) \mathcal{D}\phi_2(\vec{x}) . \int_{\substack{\phi\left(x_1^0, \vec{x}\right) = \phi_1(\vec{x}) \\ \phi\left(x_2^0, \vec{x}\right) = \phi_2(\vec{x})}} \mathcal{D}\phi(x)$$

namely introducing two specific boundary conditions at times x_1^0 and x_2^0 (in addition to those at the endpoints $-T$ and T), but integrating separately over the corresponding fixed-time field configurations $\phi_1(\vec{x})$ and $\phi_2(\vec{x})$.Consider first the case $T > x_2^0 > x_1^0 >$

$-T$. Under this time ordering, the exponential term in (3.54) can be decomposed as

$$e^{i\int_{-T}^{T} d^4x\mathcal{L}(\phi)} = e^{i\int_{-T}^{x_1^0 d^4}\, x\mathcal{L}(\phi)} \times e^{i\int_{x_1^0}^{x_2^0} d^4x\mathcal{L}(\phi)} \times e^{i\int_{x_2^0}^{T} d^4x\mathcal{L}(\phi)}.$$

After the decomposition of the main integral, the extra factors $\phi(x_1)$ and $\phi(x_2)$ in (3.54) become $\phi_1(\vec{x}_1)$ and $\phi_2(\vec{x}_2)$, and can be taken outside the inner integral. We thus obtain

$$I_{12}(x_2 > x_1) = \int \mathcal{D}\phi_1(\vec{x})\mathcal{D}\phi_2(\vec{x})\phi_1(\vec{x}_1)\,\phi_2(\vec{x}_2) \times \underbrace{\left\langle \phi_F \left| e^{-iH\left(T-x_2^0\right)} \right| \phi_2 \right\rangle}_{\int \mathcal{D}\phi e^{i\int_{x_2^0}^{T}\mathcal{L}(\phi)dx^4}} \cdot \underbrace{\left\langle \phi_2 \left| e^{-iH\left(x_2^0-x_1^0\right)} \right| \phi_1 \right\rangle}_{\int \mathcal{D}\phi e^{i\int_{x_1^0}^{x_2^0}\mathcal{L}(\phi)dx^4}} \cdot \underbrace{\left\langle \phi_2 \left| e^{-iH\left(x_1^0+T\right)\right)} \right| \phi_I \right\rangle}_{\int \mathcal{D}\phi e^{i\int_{-T}^{x_1^0}\mathcal{L}(\phi)dx^4}}. \quad (3.55)$$

$\phi(T) = \phi_F$ and $\phi(-T) = \phi_I$ .The main integral then factors into three pieces, each being a simple transition amplitude as shown above. ,Note that the times x_1^0 and x_2^0 automatically fall in order. We can turn the field $\phi_1(\vec{x}_1)$ into a Schrödinger operator using $\phi_S(\vec{x}_1)|\phi_1\rangle = \phi_1(\vec{x}_1)|\phi_1\rangle$. The completeness relation $\int \mathcal{D}\phi_1 |\phi_1\rangle\langle\phi_1| = \mathbf{1}$ then allows us to eliminate the intermediate state $|\phi_1\rangle$. Similar manipulations work for ϕ_2, yielding the expression

$$\left\langle \phi_F \left| e^{-iH\left(T-x_2^0\right)} \phi_S(\mathbf{x}_2)\, e^{-iH\left(x_2^0-x_1^0\right)} \phi_S(\mathbf{x}_1)\, e^{-iH\left(x_1^0+T\right)} \right| \phi_I \right\rangle.$$

Most of the exponential factors combine with the Schrödinger operators to make Heisenberg operators. In the case $x_1^0 > x_2^0$, the order of x_1 and x_2 would simply be interchanged. Thus expression 3.54 after similar steps becomes

$$\left\langle \phi_F \left| e^{-iHT} T\left\{\phi_H(x_1)\,\phi_H(x_2)\right\} e^{-iHT} \right| \phi_I \right\rangle.$$

This expression is almost equal to the two-point correlation function. To make it more nearly equal, we take the limit $T \to \infty(1 - i\epsilon)$. Just as in Section 3.1.4, this trick projects out the vacuum state $|\Omega\rangle$ from $|\phi_a\rangle$ and $|\phi_b\rangle$ (provided that these states have some overlap with $|\Omega\rangle$, which we assume). For example, decomposing $|\phi_a\rangle$ into

eigenstates $|n\rangle$ of H, we have

$$e^{-iHT}\left|\phi_a\right\rangle = \sum_n (e^{-iE_nT}|n\rangle \left\langle n \mid \phi_a\right\rangle)_{T\to\infty(1-i\epsilon)} \longrightarrow \left\langle \Omega \mid \phi_a\right\rangle e^{-iE_0\cdot\infty(1-i\epsilon)}.\left|\Omega\right\rangle$$

As in Section 3.1.4 , we obtain some awkward phase and overlap factors. But these factors cancel if we divide by the same quantity as (3.54) but without the two extra fields $\phi(x_1)$ and $\phi(x_2)$. Thus we obtain the simple formula

$$\left\langle \Omega \left| T\phi_H(x_1)\,\phi_H(x_2)\right| \Omega\right\rangle = \lim_{T\to\infty(1-i\epsilon)} \frac{\int \mathcal{D}\phi\phi(x_1)\,\phi(x_2)\exp\left[i\int_{-T}^{T} d^4x\mathcal{L}\right]}{\int \mathcal{D}\phi\exp\left[i\int_{-T}^{T} d^4x\mathcal{L}\right]} \tag{3.56}$$

This is our desired formula for the two-point correlation function in terms of functional integrals. For higher correlation functions, just insert additional factors of ϕ on both sides.Once we do that In general we get

$$C_n(x_1,x_2,\ldots,x_n) := \left\langle \phi(x_1)\,\phi(x_2)\cdots\phi(x_n)\right\rangle = \frac{\int \mathcal{D}\phi e^{-S[\phi]}\phi(x_1)\cdots\phi(x_n)}{\int \mathcal{D}\phi e^{-S[\phi]}} \tag{3.57}$$

For time-dependent correlation functions, the time-ordering operator T is included.

This is known as the **n -point correlation** function also called **n point greens function** in Canonical QFT.Further are gonna use it to derive our S -Matrix in Path Integral formulationin the last chapter.It should be noted that Correlation functions are also called simply correlators which can be interpreted physically as the amplitude for propagation of a particle or excitation between two space time points say y and x.

3.2.3 What are Generating Functionals in QFT?

The generating functional $\mathcal{Z}[J]$ is a key object in quantum field theory - as we shall see it reduces in ordinary quantum mechanics to a limiting form of the 1-particle propagator $G(x,x' \mid J)$ when the particle is under the influence of an external field $J(t)$. However, before beginning, it is useful to look at another closely related object, viz., the generating functional $\bar{Z}(J)$ in ordinary probability theory.

Recall that for a simple random variable ϕ, we can assign a probability distribution $P(\phi)$, so that the expectation value of any variable $A(\phi)$ that depends on ϕ is given by

$$\langle A \rangle = \int d\phi P(\phi) A(\phi)$$

where we have assumed the normalization condition

$$\int d\phi P(\phi) = 1$$

Now let us consider the generating functional $\bar{Z}(J)$ defined by

$$\bar{Z}(J) = \int d\phi P(\phi) e^{\phi} \tag{3.58}$$

From this definition, it immediately follows that the " n -th moment" of the probability distribution $P(\phi)$ is

$$g_n = \langle \phi^n \rangle = \int d\phi P(\phi) \phi^n = \left. \frac{\partial^n \bar{Z}(J)}{\partial J^n} \right|_{J=0} \tag{3.59}$$

and that we can expand $\bar{Z}(J)$ as

$$\begin{aligned} \bar{Z}(J) &= \sum_{n=0}^{\infty} \frac{J^n}{n!} \int d\phi P(\phi) \phi^n \\ &= \frac{1}{n!} g_n J^n \end{aligned} \tag{3.60}$$

so that $\bar{Z}(J)$ acts as a "generator" for the infinite sequence of moments g_n of the probability distribution $P(\phi)$

For future reference it is also useful to recall how one may also expand the logarithm of $\bar{Z}(J)$; we write,

$$\begin{aligned} \bar{Z}(J) &= \exp[\bar{W}(J)] \\ \bar{W}(J) &= \ln \bar{Z}(J) = \ln \int d\phi P(\phi) e^{\phi}. \end{aligned} \tag{3.61}$$

Now suppose we make a power series expansion of $\bar{W}(J)$, i.e.,

$$\bar{W}(J) = \sum_{n=0}^{\infty} \frac{1}{n!} C_n J^n \tag{3.62}$$

where the C_n, known as "cumulants", are just

$$C_n = \left. \frac{\partial^n \bar{W}(J)}{\partial J^n} \right|_{J=0}$$

The relationship between the cumulants C_n and moments g_n is easily found. We notice that

$$\frac{\partial \bar{W}(J)}{\partial J} = \frac{\partial \ln \bar{Z}(J)}{\partial J} = \frac{1}{\bar{Z}} \frac{\partial \bar{Z}(J)}{\partial J}$$
$$\frac{\partial^2 \bar{W}(J)}{\partial J^2} = \frac{\partial}{\partial J} \left(\frac{1}{\bar{Z}} \frac{\partial \bar{Z}(J)}{\partial J} \right) = \left[\frac{1}{\bar{Z}} \frac{\partial^2 \bar{Z}(J)}{\partial J^2} - \frac{1}{\bar{Z}^2} \frac{\partial \bar{Z}(J)}{\partial J} \right]$$

and so on. Continuing in this way, and using eq. of C_n, we can find the $\{C_j\}$ in terms of $\{g_j\}$, by expanding $\ln \bar{Z}[J] = \ln \left\{ \exp \left[\sum_n \frac{1}{n!} g_n J^n \right] \right\}$, and comparing coefficients of J^n. We then find that

$$\begin{aligned} C_1 &= g_1 \\ C_2 &= g_2 - g_1^2 \\ C_3 &= g_3 - 3g_1 g_2 + 2g_1^3, \\ C_4 &= g_4 - 3g_2^2 - 4g_1 g_3 + 12 g_2 g_1^2 - 6 g_1^4 \end{aligned}$$

and so on. Finally, note that in simple probability theory, we can make a "Legendre" transformation to change the dependent variables; if we write

$$\bar{W}(J) = \bar{\Gamma}(\phi) + J\phi$$

then in terms of the new function $\bar{\Gamma}(\phi)$, we have

$$\frac{\partial \bar{\Gamma}(\phi)}{\partial \phi} = -J$$

and we can then rewrite everything in terms of $\bar{\Gamma}(\phi)$ and its derivatives. We will see in what follows that all of these functions of simple probability theory can be put into correspondence with functionals in QFT. As we will also see, it is useful

and illuminating to explore the analogies between probability theory, field theory, and thermodynamics/ statistics mechanics.

3.2.3.1 Generating Functionals in Field theory

Suppose we are now dealing with a quantum field $\phi(x)$ in D dimensions. Then the analogue of the generating function in eq.(3.58) for ordinary probability distribution is a generating functional $\mathcal{Z}[J]$, given by

$$\begin{aligned}\mathcal{Z}[J] &= N\int D\phi A(\phi; J=0)e^{i\int d^D x J(x)\phi(x)} \\ &= N\int D\phi e^{\frac{i}{\hbar}S[\phi]}e^{i\int d^D x J(x)\phi(x)}\end{aligned} \tag{3.63}$$

and we see that the analogue of the probability distribution $P(\phi)$ is the "partition function" $\mathcal{Z}[J=0,\phi]$, i.e., the normalization factor N in the above equation is given by

$$\begin{aligned}N^{-1} &= \mathcal{Z}[J=0] = \int D\phi e^{i/\hbar S[\phi]} \equiv \int D\phi A(\phi), \\ A(\phi) &= e^{i/\hbar S[\phi]} = e^{i/\hbar\int d^D x L(\phi(x))},\end{aligned} \tag{3.64}$$

so that the analogue of the probability distribution $P(\phi)$ for a random variable to take the value ϕ is now the amplitude $A(\phi) = e^{i/\hbar S[\phi]}$ for a field to take a given configuration $\phi(x)$. We shall see later what we must write to deal with probabilities (as opposed to amplitudes) in QFT, using a kind of "double path integral" technique (recall that in ordinary QM one discusses probabilities using the density matrix, which also can be understood in terms of a double path integral).

Note also that a convergence factor has been left out of eqs.(3.61) and (3.62). Just as in ordinary QM, we need to specify which configurations are being integrated over, and with which boundary conditions. In ordinary QM, this is done by rotating the end points of the time integration to $\pm i\infty$, or by adding a term to the exponent to force the Green function $\int Dq e^{i/\hbar S[q]}$ to pick out the ground state hence we write

$$\begin{aligned}\mathcal{Z}[J] &= N\int D\phi A(\phi; J=0)e^{i/\hbar\int d^D x\left[J(x)\phi(x)+i\epsilon\phi^2(x)\right]} \\ &= N\int D\phi e^{i/\hbar\int d^D x\left[L(\phi(x))+J(x)\phi(x)+i\epsilon\phi^2(x)\right]}\end{aligned} \tag{3.65}$$

I do not go through the demonstration that this gives the desired result, since it is similar to (but more complicated than) the demonstration for ordinary Q.M.. In any case, the key point here is that

$$\mathcal{Z}[J] = \langle 0 \mid 0 \rangle_{J(x)}$$

i.e., $\mathcal{Z}[J]$ is the vacuum expectation value for the theory, under the influence of an external source J(x).

3.2.4 Time ordered Correlation functions from Generating functionals

The time-ordered correlators/correlation functions in QFT is defined by putting Time ordering in equation 3.57 as

$$G_n(x_1, \cdots, x_n) = \left\langle 0 \left| \hat{T}\left\{\phi(x_1), \cdots, \phi(x_n)\right\} \right| 0 \right\rangle = \frac{\int D\phi e^{i/\hbar S[\phi]} \phi(x_1) \cdots \phi(x_n)}{\int D\phi e^{i/\hbar S[\phi]}} \tag{3.66}$$

where the central term is the actual defination and the last integral term is the Path Integral form of the correlation function the denominator is added to normalize the result (we cannot in general assume that the function is normalised); then the corresponding power series expansion is then

$$\mathcal{Z}[J] = \sum_{n=0}^{\infty} (i/\hbar)^n \frac{1}{n!} \int dx_1 \cdots \int dx_n G_n(x_1, \cdots, x_n) J(x_1) J(x_2) \cdots J(x_n)$$

and the G_n is related to $\mathcal{Z}[J]$ by

$$G_n(x_1, \cdots, x_n) = (-ih)^n \frac{\delta^n \mathcal{Z}[J]}{\delta J(x_1) \cdots \delta J(x_n)} \bigg|_{J=0}$$

Noting that $Z(J)$ in ordinary probability theory is just the expectation value of the function $e^{\phi J}$, we see that in scalar field theory, we have

$$\mathcal{Z}[J] = \left\langle 0 \left| \hat{T}\left\{ e^{i/\hbar \int dx J(x)\phi(x)} \right\} \right| 0 \right\rangle$$

which when expanded out gives

$$\mathcal{Z}[J] = \langle 0 \mid 0 \rangle + \frac{i}{\hbar} \int d^D x \langle 0|\phi(x)|0\rangle J(x) + \frac{1}{2!} \int d^D x_1 \int d^D x_2 \left\langle 0 \left| \hat{T} \left\{ \phi\left(x_1\right) \phi\left(x_2\right) \right\} \right| 0 \right\rangle J\left(x_1\right) J\left(x_2\right) + \ldots$$

3.2.5 Path Integral Green's Functional of a scalar Quantum Field

The transition from many-body quantum physics to field theory is a transition from a finite number of degrees of freedom to an infinite number. We will perform this transition formally thus omitting in a first step all subtleties like renormalization, even ignoring the question of the sheer existence of an interacting theory.In the beginning we consider for simplicity a system of particles of mass m which is described by a neutral scalar field $\phi(x)$. Let the Lagrange density (Lagrangian) be

$$\mathcal{L} = \frac{1}{2} \left(\partial_\mu \Phi \partial^\mu \Phi - m^2 \Phi^2 \right) - V(\Phi) \tag{3.67}$$

where $V(\Phi)$denotes the self-interaction of the field. If one requires the theory to be renormalizable (in 1 time and 3 space dimensions) this interaction can only be a polynomial of the field up to degree four; a typical example is

$$V(\Phi) = \lambda \Phi^4 / 4! \tag{3.68}$$

which is of great importance in superconductivity (Ginzburg-Landau theory) and particle physics (Higgs mechanism). As in the quantum-mechanical case we consider the transition matrix element

$$\left\langle \Phi_f \left| e^{-i\hat{H}\left(t_f - t_i\right)} \right| \Phi_i \right\rangle \tag{3.69}$$

of the time-evolution operator between field configurations Φ_i and Φ_f and $H = \int d^3x \mathcal{H}$ is the Hamilton operator of the systems. The classical Hamilton density follows by the usual Legendre transformation as

$$\mathcal{H} = \pi \dot{\Phi} - \mathcal{L} = \frac{1}{2}\pi^2 + \frac{1}{2}(\nabla\Phi)^2 + \frac{1}{2}m^2\Phi^2 + V(\Phi) \tag{3.70}$$

where $\pi = \partial\mathcal{L}/\partial\Phi$ is the canonically conjugated momentum (density) of the field. We divide the (finite) space volume L^3 into N small cells with volume $v = L^3/N$ and the time interval $t_f t_i$ in M intervals of length o. If we use the completeness for the fields $Phi(t,x) = \Phi_l j$ where , l = 1 . . .M 1, j = 1 . . .N at each time and space point Z

$$\int d\Phi_j^l \left|\Phi_j^l\right\rangle \left\langle\Phi_j^l\right| = 1 \tag{3.71}$$

then we obtain

$$\left\langle \Phi_f \left| e^{-i\hat{H}\left(t_f - t_i\right)} \right| \Phi_i \right\rangle = \lim_{N,M\to\infty} \int \prod_{j=1}^{N} \left\{ d\Phi_j^{M-1} \ldots d\Phi_j^1 \left\langle \Phi_j^M \left| e^{-i\epsilon v\hat{\mathcal{H}}} \right| \Phi_j^{M-1} \right\rangle \right.$$
$$\left. \ldots \left\langle \Phi_j^1 \left| e^{-i\epsilon v\hat{H}} \right| \Phi_j^0 \right\rangle \right\}$$

ore we have set $\Phi_j^M = \Phi_f\left(\mathbf{x}_j\right)$ and $\Phi_j^0 = \Phi_i\left(\mathbf{x}_j\right)$ as abbreviation. Exactly as in the quantum mechanical case finds for small times

$$\left\langle \Phi_j^{l+1} \left| e^{-i\epsilon v\hat{H}} \right| \Phi_j^l \right\rangle \simeq \int \frac{dp_j^l}{2\pi} \exp\left[ip_j^l \left(\Phi_j^{l+1} - \Phi_j^l\right) - i\epsilon v\mathcal{H}_j^l \right]$$

If we write $p_j^l = v\pi_j^l$, we obtain

$$\begin{aligned} \left\langle \Phi_f \left| e^{-i\hat{H}\left(t_f - t_t\right)} \right| \Phi_i \right\rangle = \lim_{N,M\to\infty} & \int \prod_{j=1}^{N} \left(\prod_{l=1}^{M-1} \frac{d\Phi_j^l v d\pi_j^l}{2\pi} \right) \int \frac{v d\pi_j^M}{2\pi} \\ & \cdot \exp\left\{ i\epsilon \sum_{l=0}^{M-1} v \sum_{j=1}^{N} \left(\pi_j^l \frac{\Phi_j^{l+1} - \Phi_j^l}{\epsilon} - \mathcal{H}_j^l \right) \right\} \\ \equiv & \int \frac{\mathcal{D}\Phi(x)\mathcal{D}\pi(x)}{2\pi} \exp\left\{ i \int_{t_t}^{t_f} dt \int d^3x [\pi\dot{\Phi} - \mathcal{H}(\pi,\Phi)] \right\} \end{aligned} \tag{3.72}$$

This is the expression for **Path integral of a sclar field** in Hamilton form . By completing the square $\left(\pi\dot{\Phi} - \pi^2/2 = -(\pi - \dot{\Phi})^2/2 + \dot{\Phi}^2/2\right)$ we can transform the π -integral into a Gaussian integral and we then obtain the **Path integral in Lagrange form** as

$$\left\langle \Phi_f \left| e^{-i\hat{H}\left(t_f - t_i\right)} \right| \Phi_i \right\rangle = \text{ const. } \cdot \int \mathcal{D}\Phi(x) e^{iS[\Phi]} \tag{3.73}$$

Note: Again we have the (classical) action in the exponent of 3.71 because

$$\int_{t_t}^{t_f} dt \int d^3x \left[\frac{1}{2}\dot{\Phi}^2 - \frac{1}{2}(\nabla\Phi)^2 - \frac{1}{2}m^2\Phi^2 - V(\Phi)\right]$$
$$= \int_{t_t}^{t_f} dt \int d^3x \left[\frac{1}{2}\partial_\mu\Phi\partial^\mu\Phi - \frac{1}{2}m^2\Phi^2 - V(\Phi)\right] = \int_{t_i}^{t_f} dt \int d^3x \mathcal{L}\left(\Phi(x), \partial_\mu\Phi(x)\right) \equiv S[\Phi]$$

However, this representation of the transition matrix element between field configurations is only an intermediate step as this is not the relevant quantity in field theory. **Actually, all observables in field theory can be obtained from the n-point functions or Green functions** given by 3.64

$$G_n\left(x_1 \ldots x_n\right) = \left\langle 0 \left| \mathcal{T}\left[\hat{\Phi}\left(x_1\right) \ldots \hat{\Phi}\left(x_n\right)\right] \right| 0 \right\rangle$$

(as can be seen below in the example of scattering of two scalar particles). Here $|0\rangle$ is the exact ground state of the theory (the trivial "vacuum"), $\mathcal{T}$ the time-ordering operator and $\hat{\Phi}(x)$ are the exact field operators in the Heisenberg picture. What we need therefore is a path-integral represention for the Green functions.

Fortunately, this already has been in the previous sections for case of quantum mechanics and is not hard to generalise it to Quantum Field theory . The ground state can be projected out by the unphysical limit $t_i \to i\infty, t_f \to -i\infty$ and one has

$$G_n\left(x_1 \ldots x_n\right) = \lim_{\substack{t_i \to \infty \\ t_f \to -\infty\infty}} \frac{\int \mathcal{D}\Phi\Phi\left(x_1\right) \ldots \Phi\left(x_n\right) \exp(iS[\Phi])}{\int \mathcal{D}\Phi \exp(iS[\Phi])} \tag{3.74}$$

The set of all n-point functions of a scalar field can be obtained from the functional differentiation of **Generating functional $Z[J]$ of the scalar field** which is

$$Z[J] = \int \mathcal{D}\Phi \exp\left(iS[\Phi] + i\int d^4x J(x)\Phi(x)\right) \tag{3.75}$$

Hence G_n can be expressed as

$$G_n\left(x_1 \ldots x_n\right) = \left(\frac{1}{i}\right)^n \frac{\delta^n}{\delta J\left(x_1\right) \ldots \delta J\left(x_n\right)} \frac{Z[J]}{Z[0]}\bigg|_{J=0} \tag{3.76}$$

As one can see the normalization of the functional integral cancels. Eq. (3.73) can also be considered as functional Fourier transform of $\exp(iS[\Phi])$ and thus the artificially

introduced source $J(x)$ can be seen as variable conjugate to the field $\Phi(x)$. In most cases the generating functional can be calculated only for vanishing self-interaction V : as

$$\begin{aligned} Z_0[J] &= \int \mathcal{D}\Phi \exp\left[i \int d^4x \left(\frac{1}{2}\partial_\mu \Phi \partial^\mu \Phi - \frac{1}{2} m^2 \Phi^2 + J\Phi \right) \right] \\ &= \int \mathcal{D}\Phi \exp\left[\frac{i}{2} \int d^4x \Phi(x) \left(-\partial^2 - m^2 \right) \Phi(x) + i \int d^4x J(x)\Phi(x) \right]. \end{aligned}$$

In the second line an integration by parts has been performed under the assumption that boundary terms vanish. The functional integration in the above Eq. can be done since the exponent

$$\begin{aligned} &\frac{i}{2} \int d^4x d^4y \Phi(x) K_0(x,y) \Phi(y) + i \int d^4x J(x)\Phi(x) \\ &= \frac{i}{2} \int d^4x d^4y \left(\Phi K_0 + J \right)(x) K_0^{-1}(x,y) \left(K_0 \Phi + J \right)(y) - \frac{i}{2} \int d^4x d^4y J(x) K_0^{-1}(x,y) J(y) \end{aligned}$$

is quadratic in the fields. The Gaussian integral over Φ thus gives

$$Z_0[J] = const \cdot \exp\left[-\frac{i}{2} \int d^4x d^4y J(x) K_0^{-1}(x,y) J(y) \right] \equiv Z_0[0] \exp\left[-\frac{i}{2} \left(J, K_0^{-1} J \right) \right] \tag{3.77}$$

where the constant does not depend on the source. In addition, we have used a convenient short-hand notation. The inverse of the kernel

$$K_0(x,y) = \left(-\partial_x^2 - m^2 \right) \delta^4(x-y)$$

is calculated most easily in momentum space as - due to translational invariance $-K_0$ only depends on the difference $x - y$:

$$\Delta(x,y) \equiv K_0^{-1}(x,y) = \int \frac{d^4k}{(2\pi)^4} \tilde{\Delta}(k) e^{ik\cdot(x-y)}$$

The equation

$$\left(-\partial_x^2 - m^2 \right) \Delta(x,y) = \delta^4(x-y)$$

then just becomes an algebraic equation

$$\left(k^2 - m^2 \right) \tilde{\Delta}(k) = 1$$

with the solution

$$\tilde{\Delta}_F(k) = \frac{1}{k^2 - m^2 + i0^+} \tag{3.78}$$

This is the Feynman propagator in momentum space. Of course, one has to specify how to treat the pole at $k^2 = m^2$ this can be achieved by a more careful treatment of the limit $t_i \to i\infty, t_f \to -i\infty$ in the path-integral representation (3.74) for the Green functions, or simpler by introducing a convergence factor

$$\exp\left[-\frac{\epsilon}{2}\int d^4x \Phi^2(x)\right], \quad \epsilon > 0$$

into the path integral. By combining this term with the mass term in the Lagrangian this leads to the replacement

$$m^2 \longrightarrow m^2 - i0^+$$

($i0^+$ is a short-hand for a small, postive imaginary part $i\epsilon, \epsilon > 0$ which at the end of the calculation is set to zero.). From Eq. (3.75) one thus finds that the 2-point function (or the propagator) in lowest order is given by

$$G_2^{(0)}(x_1, x_2) = i\Delta_F(x_1, x_2) \tag{3.79}$$

The **generating functional with interaction** can be obtained formally from $Z_0[J]$ by functional differentiation. As functional differentiation w.r.t. the source $J(x)$ generates the field $\Phi(x)$ we thus have

$$\begin{aligned} Z[J] &= \int \mathcal{D}\Phi \exp\left[-i\int d^4x V\left(\frac{1}{i}\frac{\delta}{\delta J(x)}\right)\right] \exp\left[i\int d^4y \left(\mathcal{L}_0 + J(y)\Phi(y)\right)\right] \\ &= \exp\left[-i\int d^4x V\left(\frac{1}{i}\frac{\delta}{\delta J(x)}\right)\right] Z_0[J] \end{aligned} \tag{3.80}$$

3.2.5.1 Machinery of Generating Functionals:A Functional Equation for the Generating Functional

The representation of the generating functional as a functional integral offers many possibilities for transformations known from usual integral calculus. For instance, we may perform an infinitesimal shift of the integration variable

$$\Phi(x) = \varphi(x) + \epsilon f(x)$$

As the Jacobian of transformation is obviously is "1", thus we have

$$Z[J] = \int \mathcal{D}\varphi \left\{ 1 + i\epsilon \int d^4x f(x) \frac{\delta}{\delta\varphi(x)} \exp\left(iS[\varphi] + i \int d^4x J(x)\varphi(x) \right) \right\}.$$

Since the function $f(x)$ is totally arbitrary, the (functional) integral over a total (functional) derivative must vanish (as in ordinary integral calculus):

$$\begin{aligned} 0 &= \int \mathcal{D}\varphi \frac{\delta}{\delta\varphi(x)} \exp\left(iS[\varphi] + i \int d^4x J(x)\varphi(x) \right) \\ &= i \int \mathcal{D}\varphi \left\{ \frac{\delta S[\varphi]}{\delta\varphi(x)} + J(x) \right\} \exp\left(iS[\varphi] + i \int d^4x J(x)\varphi(x) \right) \end{aligned} \tag{3.81}$$

We may pull out the terms, which contain φ in the curly bracket, from the functional integral if we replace $\varphi(x)$ by $\delta/(i\delta J(x))$ (acting on the generating functional) in these terms. Then we obtain

$$\left\{ \frac{\delta S}{\delta\varphi(x)} \left[\frac{\delta}{i\delta J(x)} \right] + J(x) \right\} Z[J] = 0$$

which for the scalar theory explicitly reads

$$\left\{ \left(\partial^2 + m^2\right) \frac{\delta}{i\delta J(x)} + V'\left(\frac{\delta}{i\delta J(x)} \right) - J(x) \right\} Z[J] = 0 \tag{3.82}$$

This so-called **Schwinger equation** therefore connects different n -point functions

3.2.6 Greens function as Feynman Propagator

In this section, you will make your first acquaintance with path integral. In quantum theory, path integral is a method of constructing the propagator. So we begin with the propagator. Recall the Green's Function ,mathematically Green's function $G(x;x^{'})$ of an operator L is defined as

$$LG(x;x^{'}) = \delta(x;x^{'})$$

this method is very useful to solve equations like

$$L\varphi(x) = J(x)$$

since if we know the Green's function $G(x;x^{'})$ of L, the solution is simply

$$\varphi(x) = \int G(x;x')J(x')dx'$$

One can easily verify it notice

$$L\varphi(x) = L\int G(x;x')J(x')dx'$$

$$= \int LG(x;x')J(x')dx' = \int \delta(x;x')J(x')dx' = J(x)$$

Where the second equality is due to the fact that L consists only operation on x and is totally irrelevant to x'.

In Quantum Mechanics , we have the Schrödinger's Equation

$$\left[i\frac{\partial}{\partial t} + \frac{1}{2m}\nabla^2\right]|\psi\rangle = 0$$

All within the bracket can be be viewed as an operator, and thus possesses a Green's function

$$\left[i\frac{\partial}{\partial t} + \frac{1}{2m}\nabla^2\right]K(t,x;t',x') = \delta(x;x')\delta(t;t') \tag{3.83}$$

with this propagator , we can calculate the state of anytime after from an initial state

$$|\psi(t')\rangle = \int K(t,x;t',x')|\psi(t)\rangle dxdt \tag{3.84}$$

therefore , the initial state $|\psi(t)\rangle$ propagetes to the final state $|\psi(t')\rangle$ with the help of K(x,t;x';t'). As a consequence,K(x,t;x',t') is called the propagator.

Feynman suggest the propagator takes the form

$$K = \int \mathcal{D}x e^{iS[x]} \tag{3.85}$$

3.2.7 Perturbation theory in Path Integrals

The relation

$$Z[J] = \exp\left[-i\int d^4x V\left(\frac{1}{i}\frac{\delta}{\delta J(x)}\right)\right] Z_0[J] \tag{3.86}$$

between the Generating Functional with and without Interaction is purely a formal one and comes to use only when we expand the Interaction in terms of coupling constant of the theory. For this consider the expansion of form

$$Z[J] = Z_0[J]\left\{1 + \lambda\omega_1[J] + \lambda^2\omega_2[J] + \ldots\right\}$$

where

$$\omega_1[J] = -\frac{i}{4!}\frac{1}{Z_0[J]}\int d^4x \left(\frac{\delta}{\delta J(x)}\right)^4 Z_0[J]$$

Expanding the differentials gives

$$\begin{aligned}\omega_1[J] = -\frac{i}{4!}\int d^4x \Big\{ & 3(-i)^2\Delta_F(x,x)\Delta_F(x,x) \\ & + 6(-i)^3\int d^4y_1 d^4y_2 \Delta_F(x,y_1)\, J(y_1)\, \Delta_F(x,x)\Delta_F(x,y_2)\, J(y_2) \\ & + (-i)^4\int d^4y_1 d^4y_2 d^4y_3 d^4y_4 \prod_{j=1}^{4}\Delta_F(x,y_j)\, J(y_j)\end{aligned} \tag{3.87}$$

The different terms can be ordered according to the number of sources J and represented graphically: Each propagator $\Delta_F(x, y)$ is symbolized by a line leading from y to x and each interaction vertex by a point into which 4 lines are going in or out as shown below

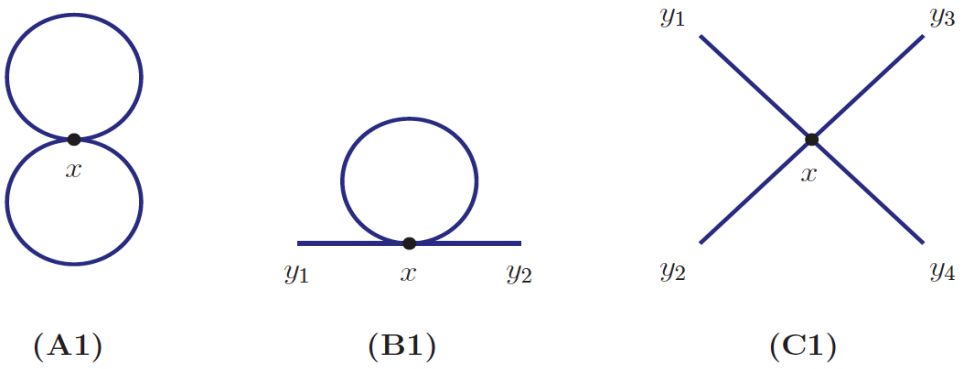

Figure 3.5: Graphical representation of first-order perturbation theory ω_1 for the generating functional in Φ^4-theory

In second-order perturbation theory one finds

$$\omega_2[J] = \frac{1}{2}\omega_1^2[J] + \tilde{\omega}_2[J]$$

where the first contribution on the r.h.s. contains disconnected graphs in which two parts are not connected by a common line (see, e.g. Fig.3.6 below where the first-order graphs (A1) and (B1) are taken together without connection).

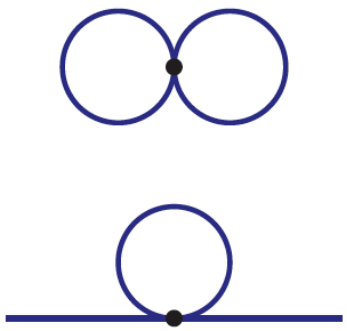

Figure 3.6: A disconnected graph in 2nd order perturbation theory for the Φ^4-theory

3.2.8 Connected and Amputated Greens Functions and their Generators

We have seen how the generating functional or partition function or vacuum expectation value $\mathcal{Z}[J]$ corresponds to the generating function $\bar{Z}(J)$ for simple probability distributions. Let us now continue this analogy, and write

$$\mathcal{Z}[J] = e^{\frac{i}{\hbar}W[J]} \tag{3.88}$$

We now proceed , by defining what we call "connected" Green functions (the name will become clear) as

$$\mathcal{G}_n^{(c)}(x_1, \ldots, x_n) = (-i\hbar)^n \frac{1}{W[J]} \frac{\delta^n W[J]}{\delta J(x_1) \cdots \delta J(x_n)}\bigg|_{J=0} \tag{3.89}$$

and

$$W[J] = -i\hbar \sum_{n=1}^{\infty} \left(\frac{i}{\hbar}\right)^n \frac{1}{n!} \int dx_1 \ldots dx_n \mathcal{G}_n^{(c)}(x_1, \cdots, x_n) J(x_1) \ldots J(x_n) \tag{3.90}$$

Composing eqs. (3.89) and (3.90), we see that

$$G_n(x_1, \ldots, x_n) = \mathcal{Z}[J]\mathcal{G}_n^{(c)}(x_1, \ldots, x_n)$$

3.2.9 Vertex Functional of Scalar Field Theory

So far we have expanded two different functionals as infinite series, i.e., the vacuum energy generating functional $\mathcal{Z}[J]$ (the partition function), and the generating functional $W[J]$ for connected diagrams (analogous to the free energy in statistics mechanics), related by

$$W[J] = -i\hbar \ln \mathcal{Z}[J] \tag{3.91}$$

with expansions

$$\mathcal{Z}[J] = \sum_n \left(\frac{i}{\hbar}\right)^n \frac{1}{n!} \prod_{j=1}^{n} \int d^D x_j G_n(x_1, \ldots, x_n) J(x_j) \tag{3.92}$$

and

$$W[J] = \sum_n \left(\frac{i}{\hbar}\right)^n \frac{1}{n!} \prod_{j=1}^{n} \int d^D x_j \mathcal{G}_n^{(c)}\left(x_1, \ldots, x_n\right) J\left(x_j\right) \tag{3.93}$$

Now we introduce a 3rd expansion, in terms of a new generating functional $\Gamma[\phi]$; this however, is not a functional of the external currents, but of the field $\phi(x)$ itself. We write

$$\Gamma[\phi] = \sum_{n=1}^{\infty} \frac{1}{n!} \int d^4 x_1 \cdots \int d^4 x_n \Gamma_n\left(x_1, \ldots, x_n\right) \phi\left(x_1\right) \ldots \phi\left(x_n\right) \tag{3.94}$$

so that

$$\Gamma_n\left(x_1, \ldots, x_n\right) = \left.\frac{\delta^n \Gamma[J]}{\delta\phi\left(x_1\right) \cdots \delta\phi\left(x_n\right)}\right|_{\phi=0} \tag{3.95}$$

Now of course the way to change variables between the $J\left(x_i\right)$ and the $\phi\left(x_i\right)$ is by a Legendre transformation, with form given here by

$$\Gamma[\phi] = W[J] - \int d^4 x J(x) \phi(x)$$

Thus now we now have the pair of relations

$$\begin{aligned} \left.\frac{\delta W[J]}{\delta J(x)}\right|_{\phi} &= \phi(x) \\ \left.\frac{\delta \Gamma[J]}{\delta \phi(x)}\right|_{J} &= -J(x) \end{aligned} \tag{3.96}$$

Vertex functions like $\Gamma_n\left(x_1, \ldots, x_n\right)$, turn out to be central to the approach of QFT to the dynamics of real physical systems - they are used in everything from scattering theory to particle physics to transport theory in condensed matter systems.

3.2.10 Relation between Connected Greens function and Vertex Functionals

Here we will simply establish the relationship between the connected Green functions $\mathcal{G}_n^{(c)}\left(x_1, \ldots, x_n\right)$ and the proper vertices $\Gamma_n\left(x_1, \ldots, x_n\right)$. Let's first do this for the simplest case, that of the 2 nd-order correlators $\mathcal{G}_2^{(c)}\left(x_1, x_2\right)$ and $\Gamma_2\left(x_1, x_2\right)$. From their

definitions, and from eq. (42), we have

$$\mathcal{G}_2^{(c)}(x_1, x_2) = -\hbar^2 \frac{\delta^2 W[J]}{\delta J(x_1)\,\delta J(x_2)}\bigg|_{J=0} = -\hbar^2 \frac{\delta\phi(x_1)}{\delta J(x_2)}\bigg|_{J=0}$$
$$\Gamma_2(x_1, x_2) = \frac{\delta^2 \Gamma[J]}{\delta\phi(x_1)\,\delta\phi(x_2)}\bigg|_{\phi=0} = -\frac{\delta J(x_1)}{\delta\phi(x_2)}\bigg|_{\phi=0}$$

from which we immediately find that

$$\int d^4y \mathcal{G}_2^{(c)}(x_1, y)\,\Gamma_2(y, x_2) = \frac{\delta\phi(x_1)}{\delta\phi(x_2)} = \hbar^2\delta(x_1 - x_2)$$

whose Fourier transform is

$$\mathcal{G}_2^{(c)}(p, -p) = \frac{-\hbar^2}{\Gamma_2(p, -p)}$$

i.e. the two functions are inverses of each other.

CHAPTER 4

S-Matrix in Path Integral Formalism

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4.1 Scattering Matrix (S-Matrix) construction in Path Integral formalism

Now we have developed all the necessary tools in order to formally construct our S-Matrix in the Path Integral as well analyse its Unitarity. We start by giving a rough sketch of how we are going to proceed.

4.1.1 Sketch of Theoretical construction

Before we step into the path integral form of S-Matrix , we give an overall sketch as well as some rules of our construction here. Beware, that the rules are not necessarily accepted or respected by all the academics.The construction will start from analyzing the general path integral of scalar field from some stable state to itself (usually it is

vacuum state $|\Omega\rangle$)

$$\langle\Omega \mid \Omega\rangle = N \int \mathcal{D}\varphi \exp\left\{-\frac{1}{2}\mathrm{i}\int \varphi\left[\partial^2 - m^2\right]\varphi\right\} = 1 \tag{4.1}$$

where N is a normalization factor. The last equality comes from the property stable, which means it will not change under the situation of free field, which will determine the normalization factor. Then, we construct a quantity called generating functional by adding an arbitrary potential J

Step 1

$$\begin{aligned} W_0[J] = \langle\Omega \mid \Omega\rangle|_J &= N \int \mathcal{D}\varphi \exp\left\{-\mathrm{i}\int \frac{1}{2}\varphi\left[\partial^2 - m^2\right]\varphi - J\varphi\right\} \\ &= \exp\left\{-\frac{1}{2}\mathrm{i}\int J\Delta_F J\right\} \end{aligned} \tag{4.2}$$

The above generating functional includes merely the scalar field without any other actual interaction terms (the J term is an auxiliary term with no physical significance). If the Lagrangian includes the interaction terms $\mathcal{L}_{\text{int}}$, the generating functional will be

Step 2

$$\begin{aligned} W[J] &= \exp\left\{-\mathrm{i}\int \mathcal{L}_{\text{int}}\left[\frac{1}{\mathrm{i}}\frac{\delta}{\delta J}\right]\right\} W_0[J] \\ &= \exp\left\{-\mathrm{i}\int \mathcal{L}_{\text{int}}\left[\frac{1}{\mathrm{i}}\frac{\delta}{\delta J}\right]\right\} \exp\left\{-\frac{1}{2}\mathrm{i}\int J\Delta_F J\right\} \end{aligned} \tag{4.3}$$

As is indicated, this expression deals with some stable state. Now we hope to generalized it into other ordinary states, like from state α to state β. This will give us the well-renowned S-matrix (scattering matrix) in P.I formulation

Step 3

$$S = \langle\beta \mid \alpha\rangle = S[J]|_{J=0} = \exp\left\{\mathrm{i}\int \varphi_{as}\left(\partial^2 - m^2\right)\frac{\delta}{\delta J}\right\} W[J]\Big|_{J=0} \tag{4.4}$$

where φ_{as} is the asymptotic field corresponding to the initial and final state. The last equality 4.4 is nothing but the famous LSZ reduction formula(but now in Path Integral formulation).

After arriving at the S-matrix, the theoretical construction will come to a conclusion. The S-matrix, which is directly observable in the scattering experiment, may be used to calculate the scattering cross-section. As previously indicated, we will not incorporate any components from canonical quantization into our development of the path integral formalism. As a result, we are unable to utilise notions such as state, which are frequently used in quantum theory. In this scenario, we'll need to employ some field setting as a state (like asymptotic field). However, this implies that there must be a subtle identical connection between field and state, which canonical quantum field theory rejects. In actuality, the difficulty caused by the lack of a field operator and consecutive state only emerges when creating an S-matrix, thus stage 1 and stage 2 are unaffected in any case. The path integral formalism, as a complement to canonical quantization in our philosophy, should be free of notions in canonical form. As a result, we'll do our best to avoid using terms like field operator and matching state, or at the very least push them as far down as feasible.

4.1.2 Free Scalar Field theory

This section will introduce the free scalar field theory, i.e. stage 1 mentioned in the sketch. Our main goal here is to derive the generating functional of the free scalar field. First we need a vacuum state as the initial and final state — just like the start and end point in path integral of Quantum Mechanics. However, the vacuum is not so straight-forward in Quantum Field Theory. We hereby define the vacuum state $|\Omega\rangle$as the configuration of field with the lowest possible energy, which is the general starting point of the term vaccum. Now, we express the probability of the free field from vacuum state to vacuum state in terms of path integral. The probability should be unity since there are no interactions. Therefore

$$W = \langle \Omega \mid \Omega \rangle = \mathcal{N} \int \mathcal{D}\varphi \exp\left\{ -\frac{1}{2}\mathrm{i} \int \varphi \left(\partial^2 - m^2 \right) \varphi \right\} = 1 \tag{4.5}$$

where we now know the normalization factor $\mathcal{N}$. We already know the Lagrangian. The scalar field is real here, and it won't be miserable to generalize this into complex situation. However, This formulation does not tell us anything except for a normalization factor, since it is trivial - from vacuum to vacuum with no interaction. Now, we want to add some interactions. To achieve this, we introduce an auxiliary potential J

and the Lagrangian becomes

$$\mathcal{L} = -\varphi\left(\partial^2 - m^2\right)\varphi + J\varphi \tag{4.6}$$

and the path integral becomes

$$W[J] = \langle\Omega \mid \Omega\rangle|_J = \mathcal{N}\int \mathcal{D}\varphi \exp\left\{-\frac{1}{2}\mathrm{i}\int \varphi\left(\partial^2 - m^2\right)\varphi - 2J\varphi\right\} \tag{4.7}$$

Now, we perform the path integral. As what we have done in Quantum Mechanics, expand the path integral according to the classical path. The classical path φ_0 satisfies

$$\left(\partial^2 - m^2\right)\varphi_0 = J, \text{ i.e. } \varphi_0 = \int \Delta_F J$$

where Δ_F is the Green's function satisfying

$$\left(\partial^2 - m^2\right)\Delta_F\left(x; x'\right) = -\delta\left(x; x'\right)$$

Warning: minus the Please about hand s side the be the sign above equation! very careful in right h of tl Consequently, we perform translation $\varphi \mapsto \varphi + \varphi_0$. In path integral, a definite path φ_0 acts just like a constant (expand the path integral according to the definition and you will see why). A brief calculation will give

$$\begin{aligned} W[J] &= \exp\left\{-\frac{1}{2}\mathrm{i}\int J\Delta_F J\right\}\cdot\mathcal{N}\int\mathcal{D}\varphi\exp\left\{-\frac{1}{2}\mathrm{i}\int\varphi\left(\partial^2 - m^2\right)\varphi\right\} \\ &= \exp\left\{-\frac{1}{2}\mathrm{i}\int J\Delta_F J\right\} \end{aligned} \tag{4.8}$$

4.1.3 Scalar field theory with Interaction

This section introduces the self-interaction theory of scalar field. As usual, the interaction is implemented as an additional interaction term $\mathcal{L}_{\text{int}}$ in Lagrangian. The interaction discussed here is assumed to satisfy the following condition It is the self-interaction, i.e. $\mathcal{L}_{\text{int}} = \mathcal{L}_{\text{int}}[\varphi]$ It has the form of polynomials. Similarly, the construction starts from the generating functional. The generating functional of an interaction

theory is

$$\begin{aligned} W[J] &= \int \mathcal{D}\varphi \exp\{\mathrm{i}S\} = \int \mathcal{D}\varphi \exp\left\{\mathrm{i}\int \mathcal{L} + \mathcal{L}_{\text{int}}[\varphi]\right\} \\ &= \int \mathcal{D}\varphi \exp\left\{\mathrm{i}\int \mathcal{L}_{\text{in}}[\varphi]\right\} \exp\left\{\mathrm{i}\int \mathcal{L}\right\} \end{aligned} \tag{4.9}$$

Next, we expand the first exponential (the one with interaction) according to definition

$$W[J] = \int \mathcal{D}\varphi \sum_{n=0}^{\infty} \frac{1}{n!}\left[\mathrm{i}\int \mathcal{L}_{\text{int}}\left[\varphi\right]\right\}\Bigg]^{n} \exp\left\{\mathrm{i}\int \mathcal{L}\right\}$$

Now, recall our first identity

$$\frac{1}{\mathrm{i}}\frac{\delta}{\delta J(x)} W_0[J] = \int \mathcal{D}\varphi\varphi(x) \exp\{\mathrm{i}S\}$$

Therefore, each $\varphi(x)$ in $\mathcal{L}_{\text{int}}\left[\varphi\right]$ can be replaced with $\delta/\mathrm{i}\delta J(x)$, as long as $\mathcal{L}_{\text{int}}\left[\varphi\right]$ is a pure polynomial of φ. In this case, we can write

$$\begin{aligned} W[J] &= \int \mathcal{D}\varphi \sum_{n=0}^{\infty} \left[\ \mathrm{i}\ \int \mathcal{L}_{\text{int}}\ \left[\frac{1}{i}\frac{\delta}{\delta J}\right]\right\}\Bigg]^{n} \exp\left\{\mathrm{i}\int \mathcal{L}\right\} \\ &= \sum_{n=0}^{\infty} \frac{1}{n!}\left[\ \mathrm{i}\ \int \mathcal{L}_{\text{int}}\ \left[\frac{1}{i}\frac{\delta}{\delta J}\right]\right\}\Bigg]^{n} \int \mathcal{D}\varphi \exp\left\{\mathrm{i}\int \mathcal{L}\right\} \end{aligned}$$

where expression $\mathcal{L}_{\text{int}}\left[\delta/\mathrm{i}\delta J\right]$ represents the the expression where all φ in $\mathcal{L}_{\text{int}}$ is replaced with $\delta/\mathrm{i}\delta J(x)$. The terms after the replacement no longer contain φ and thus can be moved out of the path integral. And we find now that the path integral gives the generating functional $W_0[J]$ of free field. Transform back into the exponential form and we get

$$W[J] = \exp\left\{-\mathrm{i}\int \mathcal{L}_{\text{int}}\ \left[\frac{1}{\mathrm{i}}\frac{\delta}{\delta J}\right]\right\} W_0[J] \tag{4.10}$$

which is the result of second stage of our construction. The interaction of other kinds of fields (except for vector field in gauge theories) can be performed through similar manner.

4.1.4 Scattering Matrix

Scattering matrix, or S-matrix, is one of the major and core concept in both Particle and High Energy Physics - since this is the most straight-forward way to verify the form of interaction.

As we have already seen that the S-matrix is defined as an infinite dimensional matrix with each matrix element $S_{\beta\alpha}$ being the probability of the state evolving from α to β, i.e.

$$S_{\beta\alpha} = \langle \beta \mid \alpha \rangle$$

Note: As a matter of fact, the S-matrix is not a typical "matrix". It is just a quantity with each one of them can be labelled by two indices. Also, in canonical quantization, S-matrix is actually an operator which, if it is finite dimensional, can be expressed as a matrix (but in Quantum Field Theory it is not). Therefore, when you see some concept which is a matrix, it might not mean to be a typical matrix, but some operator or quantity of two indices. In Quantum Field Theory (as well as Particle Physics), we are especially interested in the following situation Two or more beams of free particle are generated and targeted at some point, interact with each other at the limited region near the point, then leave the interaction region, become free particles again and finally detected by the particle detectors. The key point in the above picture is that the interaction only happens at a restricted region, and the particles are free outside the region. This approximation can be pretty accurate if the region is selected wisely so that the particles are separated by a considerably long distance. And it is prevalently implemented in many particle colliders.

The above picture suggests us write the field in the path integral as the addition of an "interact field" φ and a free asymptotic field φ_{as} , i.e. perform the following variable translation in the path integral

$$\varphi \mapsto \varphi + \varphi_{as}$$

where the asymptotic field φ_{as} satisfies

$$\left(\partial^2 - m^2\right) \varphi_{\text{as}} = 0$$

Therefore, the S-matrix with auxiliary field J supplied is

$$S_0[J] = \int \mathcal{D}\varphi \exp\left\{-\mathrm{i}\int \frac{1}{2}\varphi\left[\partial^2 - m^2\right]\varphi - J\varphi - J\varphi_{\mathrm{as}}\right\} = \exp\left\{\mathrm{i}\varphi_{\mathrm{as}}J\right\} W_0[J] \quad (4.11)$$

Similar formula also holds for situation with interaction. Then, just as what we have done in the last section, expand the exponential as Taylor series

$$S[J] = \sum_{n=0}^{\infty} \frac{1}{n!}\left[\mathrm{i}\varphi_{\mathrm{as}}J\right]^n W[J]$$

Recall we have our second identity

$$\left(\partial^2 - m^2\right)\frac{1}{\mathrm{i}}\frac{\delta}{\delta J(x)}W_0[J] = J(x)W_0[J]$$

This inspires us that we can replace every J in the Taylor series with $\left(\partial^2 - m^2\right)\delta/\mathrm{i}\delta J$. Hence

$$S[J] = \sum_{n=0}^{\infty}\frac{1}{n!}\left[\mathrm{i}\varphi_{\mathrm{as}}\left(\partial^2 - m^2\right)\frac{1}{\mathrm{i}\delta J}\right]^n W[J] = \exp\left\{\mathrm{i}\varphi_{\mathrm{as}}\left(\partial^2 - m^2\right)\frac{1}{\mathrm{i}}\frac{\delta}{\delta J}\right\} W[J]$$

To obtain the S-matrix, simply set the auxiliary field J as zero

$$S = \exp\left\{i\varphi_{as}\left(\partial^2 - m^2\right)\frac{1}{\mathrm{i}}\frac{\delta}{\delta J}\right\} W[J]\Big|_{J=0} \quad (4.12)$$

This is the so-called **LSZ reduction formula**, which gives the S-matrix with inbound and outbound state designated by asymptotic field φ_{as} from the generating functional.

4.1.4.1 S-Matrix in Terms of Correlation Function

Recall that the Correlation function that we studies in the last chapter can be expressed here as

$$\tau\left(x_1, \ldots, x_n\right) := \frac{1}{\mathrm{i}\delta J\left(x_1\right)} \cdots \frac{1}{\mathrm{i}}\frac{\delta}{\delta J\left(x_n\right)}W_0[J]\Big|_{J=0}$$

which is the correlation function, or n -point (Green's) function. The origin of this name comes from the similarity of its formulation in canonical quantization and hence this name may look strange here. It is not so straight-forward about the n -point

function, and thus we hope to reduce the formula. To do this, let us first evaluate the 2-point function

$$\begin{aligned}\tau(x_1,x_2) &= \frac{1}{\mathrm{i}}\frac{\delta}{\delta J(x_1)}\frac{1}{\mathrm{i}}\frac{\delta}{\delta J(x_2)}\exp\left\{-\frac{1}{2}\mathrm{i}\int J\Delta_F J\right\}\Big|_{J=0}\\ &= \mathrm{i}\frac{\delta}{\delta J(x_1)}\int \Delta_F(x_2;)\,J\exp\left\{-\frac{1}{2}\mathrm{i}\int J\Delta_F J\right\}\Big|_{J=0}\\ &= \mathrm{i}\Delta_F(x_1;x_2)\,W_0[J]|_{J=0}+\left(\int \Delta_F J\right)^2 W_0[J]\Big|_{J=0} = \mathrm{i}\Delta_F(x_1;x_2)\end{aligned}$$

It is nothing other than i times the ordinary Green's function. Next, 3 -point function

$$\tau(x_1,x_2,x_3)\sim\Delta_F\int\Delta_F J\Big|_{J=0}+\left(\int\Delta_F J\right)^3\Big|_{J=0}=0$$

And 4-point function

$$\begin{aligned}\tau(x_1,x_2\cdot x_3,x_4) &= \mathrm{i}\Delta_F(x_1;x_2)\,\mathrm{i}\Delta_F(x_3;x_4)\\ &+\mathrm{i}\Delta_F(x_1;x_3)\,\mathrm{i}\Delta_F(x_2;x_4)\\ &+\mathrm{i}\Delta_F(x_2;x_3)\,\mathrm{i}\Delta_F(x_1;x_4)\\ &=(1\sim2)(3\sim4)+(1\sim3)(2\sim4)+(2\sim3)(1\sim4)\end{aligned}$$

where we have used $(1\sim 2)$ to represent $\tau(x_1,x_2)$. Therefore, we can see the regularity $-$ the n -point function is either 0 or some combination of two point functions. Specifically, we have by induction The odd-point function is 0. The even-point function is

$$\tau(x_1,\ldots,x_{2n})=\sum_{\text{verms}}(p_1\sim p_2)\ldots(p_{2n-1}\sim p_{2n})$$

which means the summation over all the permutations p. This is the so-called Wick's Theorem - transforming the n -point function into the combination of 2 -point function. It can be easily shown that the S-matrix can be written using correlation function as

$$S=\sum_{n=0}^{\infty}\frac{\mathrm{i}^n}{n!}\prod_x\varphi(x)\prod_x\left(\partial^2-m^2\right)\tau(x_1,\ldots,x_n) \tag{4.13}$$

where x takes over $x_1,\ldots,x_n$. This formula is the so-called **perturbative expansion of the S-matrix in Path integral formulation**.

4.1.5 First glance at Infinities

This section will show you how the infinities emerge in Quantum Field Theory through a resonated toy of physicists $-\varphi^4$ theory. The interaction term of φ^4 theory is

$$\mathcal{L}_{\text{int}} = -\frac{1}{4!}g\varphi^4 \tag{4.14}$$

Recall that the generating functional of interaction theory is

$$W[J] = \exp\left\{-\mathrm{i}\int \mathcal{L}_{\text{int}}\left[\frac{1}{\mathrm{i}}\frac{\delta}{\delta J}\right]\right\} W_0[J]$$

Suppose the interaction is weak enough for us to neglect all terms of order higher than one. Therefore, the generating functional up to the first order is

$$W^{(1)}[J] = \left(1 - \mathrm{i}\int \mathcal{L}_{\text{int}}\left[\frac{1}{\mathrm{i}}\frac{\delta}{\delta J}\right]\right\}\right) W_0[J] = \left(1 - \frac{\mathrm{i}g}{4!}\int \left[\frac{1\delta}{\mathrm{i}\delta J}\right]^4\right\}\right) W_0[J]$$

Notice that in this case the four functional derivatives are at the same point x. Therefore, a calculation similar to the previous section will show

$$\frac{1}{\mathrm{i}}\frac{\delta}{\delta J(x)}\frac{1}{\mathrm{i}}\frac{\delta}{\delta J(x)} W_0[J] = \tau(x,x) = \mathrm{i}\Delta(x;x) \text{ ???}$$

We see that the right hand side contains the value of Green's function at zero, which is clearly infinity. With higher order terms which contains even more derivatives, there might be even more infinities. To deal with this infinities, we use a mathematical technique called renormalization. Looking back to where the infinities come and we find

$$\frac{1}{\mathrm{i}}\frac{\delta}{\delta J(x)}\left(-\int \Delta_F(x;y)J(y)\mathrm{d}y\right)$$

makes no sense, since the functional derivative requires that $\Delta_F(x;y)$ be a function, but it is essentially a distribution (or generalized function). But things are not so bad. The Green's function is a distribution which usually has a function correspondence, and for most of the physical equations that we care, it has.

Nonetheless, the function corresponding to $\Delta(x;y)$ has no definition on $x = y$. Therefore, the above expression hopes to get something undefined. This makes things much

easier. If it is undefined, the most straight-forward way is to place an additional definition.

The renormalization procedure does exactly this stuff. Usually, we will impose some conditions (such as define the physical mass as the square-root of minus zero-point of two-point convex function) so that the value $\Delta(x; x)$ can be defined.

CHAPTER 5

S-Matrix and Quantization of Gravity

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5.1 Problem of Quantum Gravity

Reconciliation of quantum mechanics with gravity may well be the most profound theoretical problem left unsolved by twentieth-century physics. Both general relativity and quantum mechanics became well established in the first quarter of the last century, yet their clash continues to this day. One might simply declare the problem too difficult, and move on to more modest goals. But, there are glimmers of hope, both from new approaches to the problem, and perhaps more importantly, through a better understanding of the nature of the underlying difficulty. There are a number of sub-problems to that of quantizing gravity. A list includes:

1. The problem of UV divergences and nonrenormalizability: what structure cures an apparent infinite proliferation of perturbative ultraviolet divergences, and needed counterterms?

2. The problem of singularities: how can a quantum theory resolve singularities of the classical theory, such as are found in black holes and in many cosmologies?

3. The problem of observables/time: how can one formulate gauge invariant observables in the quantum theory, given that diffeomorphisms are gauge transformations in the classical theory?

4. The problem of unitarity: what dynamics unitarizes amplitudes, in the high-energy regime?

5. The conundrums of cosmology: this includes the problem of defining infrared finite observables in inflationary cosmology – an extreme example is the measure problem; or, perhaps we need an alternative to inflation.

Historically, there has been a lot of focus on problems one and two, and they have strongly motivated approaches to quantum gravity such as string theory and loop quantization. However, there are increasing indications that problems three through five are both more profound, and are linked; they seemingly drive more deeply at the heart of the central problem of quantum gravity. Indeed, there has been a growing appreciation of the fact that there are deep long distance issues in quantum gravity, which do not appear easily resolved by short-distance modifications of the theory. This suggests that a successful theory must incorporate more radical departures from local quantum field theory (QFT), relevant over even very long distance scales, in certain circumstances.

5.1.1 Approaches to Quantum Gravity

The quest for quantum gravity can be separated into three main lines of research. The relative weight of these lines has changed, there have been important intersections and connections between the three, and there has been research that does not fit into any of the three lines. Nevertheless, the three lines have maintained a distinct individuality across 70 years of research. They are often denoted "covariant," "canonical," and "sum over-histories," even if these names can be misleading and are often used interchangeably. They cannot be characterized by a precise definition, but within each line there is a certain methodological unity, and a certain consistency in the logic of the development of the research. Despite the fact that general relativity has been

present for almost more than 100 years,and have passed the subsequent test of time as well still most physicists have indeed agreed that it cannot be the ultimate theory of gravity.This is because of astounding success of the Standard Model and the Quantum Field theories that lie underneath the standard model.These theories which includes both abelian and non abelian groups has been verified experimentally to a level of precision that the Generel relativity cannot match. Another straightforward reasons include the breakdown of GTR in the vicinity of black holes and the singularities given by the theory. It is also a fully classical theory, whereas all other physics theories are quantum mechanical in nature.On the observational side, we now have extremely precise verifications of general-relativistic effects in the solar system, as well as rather compelling evidence for strong-field predictions like black holes and the "big bang." While some unproven conjectures remain, such as cosmic censorship, the development of new mathematical techniques has given us a fairly complete qualitative understanding of the theory, while computer advances have enabled us, at least in theory, to make quantitative predictions to any desired order of accuracy. The final argument, however, remains valid: despite a great deal of effort (and some results), we still lack a suitable quantum theory of gravity whose classical limit is general relativity. This is most likely today's most significant unresolved topic in theoretical physics.

Historically There are three main ways of quantizing the classical gravitational field theory.

- The **covariant line of research** is the attempt to build the theory as a quantum field theory of the Perturbative fluctuations of the metric over a flat Minkowski space, or some other background metric space. The program was started by Rosenfeld, Fierz and Pauli in the thirties. The Feynman rules of GR were laboriously found by DeWitt, Feynman and Faddeev in the sixties. t'Hooft and Veltman, Deser and Van Nieuwenhuizen, and others, found increasing evidence of nonrenormalizability at the beginning of the seventies. Then, a search for an extension of GR giving a renormalizable or finite perturbation expansion started. Through high-derivative theory and supergravity, the search converged successfully to string theory in the late eighties.

- The second method is the **canonical approach** in which one introduces a family of spacelike surfaces and constructs a Hamiltonian (eg ADM formalism of General Relativity).In this formalism the Hilbert space carries a representation of the

operators corresponding to the full metric, or some functions of the metric, without any background metric to be fixed. The program was initiated by Bergmann and Dirac in the fifties. Unraveling the canonical structure of GR turned out to be laborious. Dirac, Bergmann and his group, and Peres completed the task in the fifties. Their cumbersome formalism was drastically simplified by the introduction of new variables: first by Arnowit Deser and Misner in the sixties and then by Ashtekar in the eighties. The formal equations of the quantum theory were written down by Wheeler and DeWitt in the middle sixties, but turned out to be too ill defined. A well defined version of the same equations was successfully found only in the late eighties, with the formulation of LQG. Although many people favor this, the division into space and time seems to be contrary to the whole spirit of relativity. Also it is not clear that the concept of a spacelike surface has any meaning in quantum gravity since one would expect that there would be large quantum fluctuations of the metric on small length scales. Further, we shall want to consider topologies of the spacetime manifold that do not permit any well-behaved families of surfaces let alone spacelike ones.

- Third one is the **"Path Integral Approach"** also known as the sum-over-histories line of research is the attempt to use some version of Feynman's functional integral quantization to define the theory. The idea was introduced by Misner in the fifties, following a suggestion by Wheeler, and developed by Hawking in the form of euclidean quantum gravity in the seventies. Most of the discrete (lattice-like, posets, . . .) approaches and the spinfoam formalism, introduced more recently, belong to this line as well For these reasons we prefer the path-integral approach though it too has problems concerning the measure and the very meaning of the integral.But still this method seems to be the most fundamental one as we have seen its success in the other quantum theories.

Now we will briefly discuss all three above mentioned major approaches and we will construct and discuss the behaviour of the S-Matrix in all these formulations and analyse the Unitarity and analiticity ,thus giving us an idea of which one of these approaches seems most promising, since Unitarity is one of the most important criterion for any theory to be physically consistent.We start with a brief review of the gauge theory of gravity whose gauge symmetries are volume preserving diffeomorphisms.

5.1.2 Gauge Theory of the Group of Volume Preserving Diffeomorphisms

Given our difficulties with gravity, it is important to understand what are sharply formulated questions. One might naïvely expect that a theory of quantum gravity should calculate correlation functions − as in QFT - such as

$$\langle \phi(x)\phi(y)\cdots\rangle, \langle g_{\mu\nu}(x)\rangle\,, \langle \phi(x)\phi(y)g_{\mu\nu}(z)\cdots\rangle\,, \quad \text{etc.} \tag{5.1}$$

where ϕ is some matter field, and $g_{\mu\nu}$ is the metric. However, such correlators cannot be gauge invariant, and hence physical.**The reason is that the gauge symmetries of gravity, at least at the semiclassical level, are diffeomorphisms**, whose infinitesimal forms act on local fields by

$$\delta\phi(x) = \xi^\mu\partial_\mu\phi(x), \delta g_{\mu\nu}(x) = \nabla_{(\mu}\xi_{\nu)}(x), \text{ etc.} \tag{5.2}$$

In field theory, local observables are given in terms of the fundamental fields; but in gravity, by this reasoning, no local observables can be gauge invariant. To explore an alternative route to a viable field theory of gravitation let us go back to the very fundament - namely the two experimental observations that (1) the inertial and gravitational masses of a physical body are numerically equal, $m_I = m_G$, and that (2) the inertial energy momentum of a closed physical system is conserved, p^μ_I = conserved. Taking both together we then can write in the rest frame of the body

$$p^\mu_I = (m_I, \underline{0}) \overset{(1)}{=} (m_G, \underline{0}) = p^\mu_G \tag{5.3}$$

where we have tentatively introduced the gravitational energy-momentum p^μ_G which we keep as an entity a priorily different from p^μ_I. Note that p^μ_G is conserved due to Eqn.(5.3).

In GR $m_I = m_G$ is interpreted as an essential identity which leads to the usual geometrical description of gravitation.

We follow a different route and investigate the consequences of viewing m_I and m_G or p_I^μ and p_G^μ as different by their very natures - the prevailing view before Einstein which comes at the price of accepting the observed numerical equality $m_I = m_G$ as accidential.

Both p_I^μ and p_G^μ are four-vectors which are conserved, but in our approach through two different mechanisms. Obviously the conservation of p_I^μ is related to translation invariance in space-time. Let us use Noether's theorem to separately derive the conservation of a new four-vector in a field theoretical framework relating it to an inner continous symmetry of the theory specified below as invariance under volume-preserving diffeomorphisms. That four-vector is then interpreted as the gravitational energy-momentum p_G^μ.

To mathematically implement the idea we start with infinitesimal diffeomorphisms

$$X^\alpha \longrightarrow X'^\alpha = X^\alpha + \mathcal{E}^\alpha(X), \alpha = 0, 1, 2, 3 \tag{5.4}$$

acting on $\mathbf{R}^4$ with points labelled by $X^\alpha . X'^\alpha(X)$ denotes an infinitesimal invertible and differentiable coordinate transformation of $\mathbf{R}^4$ and $DIFF\mathbf{R}^4$ acts as a group on this space under composition.

To represent this group on fields we have to add the necessary degrees of freedom to the fields in question. So let us take a general matter field ϕ which has to be defined for our purposes on the product of the usual fourdimensional Minkowski space-time $\mathbf{M}^4$ and the four-dimensional inner space $\mathbf{R}^4$ introduced above

$$\phi(x) \to \phi(x, X)$$

with Lagrangian

$$L_M = \int d^4 X \Lambda^{-4} \mathcal{L}_M \left(\phi, \partial_\mu \phi\right) \tag{5.5}$$

Here, we have introduced a length scale Λ which is necessary to define an appropriate summation over the field components continuosly labelled by X. This summation mea-

sure has to be dimensionless as is the summation over the field components discretely labelled in the usual case of compact gauge groups - hence the necessity to introduce a length scale Λ so that $\int d^4X\Lambda^{-4}$ is dimensionless.

To next represent the group $DIFF\mathbf{R}^4$ on the matter field we take the passive view of diffeomorphisms

$$\begin{aligned} x^\mu \longrightarrow x'^\mu = x^\mu, \quad X^\alpha \longrightarrow X'^\alpha = X^\alpha \\ \phi(x,X) \longrightarrow \phi'(x,X) = \phi(x,X) - \mathcal{E}^\alpha(X)\cdot\nabla_\alpha\phi(x,X) \end{aligned} \tag{5.6}$$

transforming fields, but not coordinates. Defining the variation $\delta_\varepsilon \cdot . \equiv ..' - ..$ of an expression under an infinitesimal diffeomorphism or gauge transformation we find

$$\delta_\varepsilon L_M = -\int d^4X\Lambda^{-4}\nabla_\alpha\cdot\left(\mathcal{E}^\alpha(X)\mathcal{L}_M\left(\phi,\partial_\mu\phi\right)\right) = 0 \tag{5.7}$$

provided that the infinitesimal gauge parameter $\mathcal{E}^\alpha(X)$ is divergence-free

$$\nabla_\alpha\mathcal{E}^\alpha(X) = 0$$

This condition reduces the gauge group to volume-preserving diffeomorphisms $\overline{DIFF}\mathbf{R}^4$ which we will work with in the sequel. It is easily shown to be a group and restricts the $\mathcal{E}^\alpha(X)$ to be divergence-free.

For the Lagrangian Eqn.(5.5) Noether's theorem then yields for any solution of the field equation four conserved currents

$$\begin{aligned} J^\nu_\alpha(x) \equiv \int d^4X\Lambda^{-4}\frac{\partial\mathcal{L}_M}{\partial\left(\partial_\nu\phi\right)}\nabla_\alpha\phi \\ \partial_\nu J^\nu_\alpha(x) = 0, \alpha = 0,1,2,3 \end{aligned} \tag{5.8}$$

and four time-independent charges which is the looked-for conserved inner four-vector generating global inner coordinate transformations in field space. After gauging the current Eqn.(5.8) will serve as the source of the corresponding gauge field. Note that the above construction is transferable to any other given matter field. For clarity a comparison with the usual Yang-Mills situation might help. In our approach the theory being invariant under volume-preserving diffeomorphisms comes along with gravitational mo-

mentum conservation - accounted for by field theory means and Noether's law in analogy to how the conservation of e.g. colour in QCD is accounted for through an SU(3) global symmetry. In our case, however, the fields live on an infinitedimensional space labelled by a continous index X and not as in the QCD case on a three-dimensional vector space labelled by a discrete index.The global inner symmetry yields through Noether's theorem the conservation of gravitational momentum, gauging it leads to the gauge fields to which we turn next To obtain these we next allow for x-dependent infinitesimal volumepreserving gauge parameters $\mathcal{E}^\alpha(X) \to \mathcal{E}^\alpha(x,X), \nabla_\alpha \mathcal{E}^\alpha(x,X) = 0$. Note that Eqns.(5.6) still define the representation of the gauge group in field space.

To ensure the local gauge invariance of the Lagrangian Eqn.(5.5) we have to replace ordinary derivatives by covariant ones $\partial_\mu \to D_\mu$

$$D_\mu(x,X) \equiv \partial_\mu + A_\mu{}^\alpha(x,X) \cdot \nabla_\alpha \tag{5.9}$$

thereby introducing gauge fields $A_\mu{}^\alpha(x,X)$ which are divergence-free

$$\nabla_\alpha A_\mu{}^\alpha(x,X) = 0 \tag{5.10}$$

consistent with $\nabla_\beta \mathcal{E}^\beta(x,X) = 0$. The transformation law for the gauge field is easily derived

$$\delta_\mathcal{E} A_\mu{}^\alpha = \partial_\mu \mathcal{E}^\alpha + A_\mu{}^\beta \cdot \nabla_\beta \mathcal{E}^\alpha - \mathcal{E}^\beta \cdot \nabla_\beta A_\mu{}^\alpha \tag{5.11}$$

and respects $\nabla_\alpha \delta_\varepsilon A_\mu{}^\alpha = 0$. By construction we find the Lagrangian Eqn.(5.5)

$$\delta_\varepsilon L_M(\phi, D_\mu\phi) = -\int d^4X \Lambda^{-4} \nabla_\alpha \left(\mathcal{E}^\alpha(x,X) \cdot \mathcal{L}_M(\phi, D_\mu\phi)\right) = 0 \tag{5.12}$$

to be invariant under local gauge transformations. The field strength components are defined as usual by

$$[D_\mu(x,X), D_\nu(x,X)] \equiv F_{\mu\nu}{}^\alpha(x,X) \cdot \nabla_\alpha. \tag{5.13}$$

They are expressed by the gauge fields as

$$\begin{aligned} F_{\mu\nu}{}^{\alpha}(x,X) &= \partial_\mu A_\nu{}^{\alpha}(x,X) - \partial_\nu A_\mu{}^{\alpha}(x,X) \\ &+ A_\mu{}^{\beta}(x,X)\cdot\nabla_\beta A_\nu{}^{\alpha}(x,X) - A_\nu{}^{\beta}(x,X)\cdot\nabla_\beta A_\mu{}^{\alpha}(x,X) \end{aligned} \tag{5.14}$$

and transform covariantly under a local gauge transformation

$$\delta_{\mathcal{E}} F_{\mu\nu}{}^{\alpha} = F_{\mu\nu}{}^{\beta}\cdot\nabla_\beta\mathcal{E}^{\alpha} - \mathcal{E}^{\beta}\cdot\nabla_\beta F_{\mu\nu}{}^{\alpha}. \tag{5.15}$$

Finally, a gauge-invariant, minimal and renormalizable Lagrangian for the gauge field is given by

$$\begin{aligned} \mathcal{L}_G\left(A_\mu{}^{\alpha}, \partial^\nu A_\mu{}^{\alpha}; \nabla_\beta A_\mu{}^{\alpha}\right) &= \frac{1}{4\Lambda^2} F_{\mu\nu}{}^{\alpha}(x,X)\cdot F^{\mu\nu}{}_{\alpha}(x,X) \\ L_G &= \int d^4X \Lambda^{-4} \mathcal{L}_G\left(A_\mu{}^{\alpha}, \partial^\nu A_\mu{}^{\alpha}; \nabla_\beta A_\mu{}^{\alpha}\right) \end{aligned} \tag{5.16}$$

5.1.3 Covariant approach and the S-Matrix

A starting point for discussing the gravitational S-matrix is the observation that, to a very good approximation, Minkowski space looks like a good solution of the theory of quantum gravity. Indeed, the curvature radius of the observed Universe is of order 10^{60} in Planck units - flat space is an excellent approximation for all but the longest-scale questions, and we therefore assume that it makes sense to consider the exactly flat limit.

Next, we also observe that there are excitations about this which we describe as "particle" states, such as electrons, photons, etc., whatever their more fundamental description may be. Their asymptotic states are described by their momenta p_i, and other quantum numbers. Moreover, we can consider asymptotic multi-particle states, consisting of widely separated particles. And, in a quantum theory, we can ask for the amplitudes to transition from a given such "in" state, in the far past, to another "out" state, in the far future. This collection of amplitudes, which we might denote

$$S\left(p_{i'}, p_i\right) = {}_{\text{out}}\ \langle p_{i'} \mid p_i \rangle_{\text{in}}\ , \tag{5.17}$$

is the S-matrix. We should note there are two technicalities that we are glossing over. First, for gravity in $D = 4$ spacetime dimensions, these amplitudes aren't well-defined: instead we must perform a sum over soft gravitons, like with soft photons in QED. However, as we will see, this technicality can be avoided in higher dimensions. Secondly, a more precise definition of the S-matrix involves a map between normalizable Hilbert-space states; momentum-space states give a singlular limit of these, though one whose handling is well-understood in asymptotically flat spacetimes.

Such an S-matrix, which is tightly constrained by properties such as unitarity and analyticity, can be a very powerful way to summarize our ignorance of a theory. The S-matrix approach is so powerful that it lead to the discovery of string theory: Veneziano guessed amplitudes satisfying additional "duality" properties, and they were then found to describe excitations of one-dimensional objects. We might anticipate that such study in the context of gravity, supplemented by additional physical input, could bear important fruit.

There are multiple proposed approaches to quantizing gravity, and the S-matrix also provides a very important test for these: any theory of quantum gravity should give us a means to calculate S, at least approximately, or must provide us with some alternative physical quantities.

This test becomes particularly incisive in the ultraplanckian regime, at center of mass energies $E \gg M_D$, where M_D denotes the D-dimensional Planck mass. That any theory of quantum gravity must describe this regime follows from very general principles, and avoiding this regime appears to require radical assumptions. The first principle is that of Lorentz invariance: the Minkowski-space solution is invariant under boosts, and we can perform an arbitrarily large boost on a single-particle excitation of it to get a state with an arbitrarily large energy. The second principle is a very weak notion of locality: one can consider independently boosted particles at very large separations, and so prepare a state with a large center of mass energy – and the then allow the particles to collide. Plausibly during the big bang particles reached such energies, and it is interesting to ask whether such collisions are likely to take place anywhere in nature today. We observe that cosmic ray accelerators (argued to be active galactic nuclei) produce particles up to 1012 GeV, and now and then they could collide; that is only short by O(107). Even more interestingly, in scenarios with large and/or strongly warped extra dimensions, the fundamental Planck mass MD could be as low as the TeV range, and

in the most optimistic scenarios black holes could give important signatures at LHC While we won't talk about this phenomenology, there are multiple reviews, including. Whether or not this physics is experimentally accessible, the gedanken experiment and theoretical problem remain: we need a calculational framework that makes predictions in the ultraplanckian regime. As I will describe, here an apparently critical and fundamental problem is unitarity. However, as viewed through the lens of earlier attempts to quantize gravity, a more basic concern is that of nonrenormalizability. We will begin to understand this problem, and then explore the apparently more fundamental issue of unitarity, starting with the perturbative approach to gravity

5.1.3.1 Perturbative quantization and the Born amplitude

A starting point for perturbative quantization is the action,

$$S = \int d^D x \sqrt{-g} \left[\frac{1}{16\pi G_D} \mathcal{R} + \mathcal{L}_M \right] \tag{5.18}$$

where $\mathcal{R}$ is the Ricci scalar, $\mathcal{L}_M$ the matter lagrangian, and Newton's constant G_D is related to M_D by the Particle Data Book convention:

$$M_D^{D-2} = (2\pi)^{D-4} / (8\pi G_D) .$$

For simplicity we will typically consider for matter a minimally-coupled scalar of mass m,

$$\mathcal{L}_m = -\frac{1}{2}(\nabla\phi)^2 - \frac{1}{2}m^2\phi^2. \tag{5.19}$$

We investigate perturbations about Minkowski space,

$$g_{\mu\nu} = \eta_{\mu\nu} + \sqrt{32\pi G_D} h_{\mu\nu}$$

and expand in powers of h. This gives an action of the form

$$S = S_{m,0} + \int d^D x \left\{ \frac{1}{2} h^{\mu\nu} (\hat{\mathcal{L}} h)_{\mu\nu} + \sqrt{8\pi G_D} \left[h^{\mu\nu} T^{m,0}_{\mu\nu} + \mathcal{L}_3(h) \right] + \cdots \right\} \tag{5.20}$$

Here, quantities evaluated with $g = \eta$ are labeled with zeros, $\hat{\mathcal{L}}$ is a second-order

differential operator (a tensor analog of the laplacian), indices are raised and lowered with η, T is the stress tensor, and $\mathcal{L}_3$ is the third-order term in h. The ellipses contain higher powers of ϕ and h. The propagators are given by inverting the kinetic operators for ϕ and h; the latter requires gauge fixing. There are two approaches to this, both using the quantity

$$\bar{h}_{\mu\nu} = h_{\mu\nu} - \frac{1}{2}\eta_{\mu\nu}h^{\lambda}_{\lambda}. \tag{5.21}$$

The first is to apply the gauge fixing condition

$$\partial^{\mu}\bar{h}_{\mu\nu} = 0 \tag{5.22}$$

Alternately, one may add a gauge fixing term

$$\mathcal{L}_{gf} = \frac{1}{16\pi G_D \alpha}\left(\partial^{\mu}\bar{h}_{\mu\nu}\right)^2$$

to the lagrangian; particularly nice simplifications occur for $\alpha = -1$. In either case, one straightforwardly finds the propagator, and using that can immediately calculate a first amplitude, that for tree-level scattering of two matter particles. This is the Born amplitude. It is most conveniently given in terms of the Mandelstam invariants; let p_1, p_2 denote the momenta of the incoming particles, and $-p_3, -p_4$ those for outgoing, and define

$$s = -\left(p_1 + p_2\right)^2 = E^2, t = -\left(p_3 + p_1\right)^2 = -q^2, u = -\left(p_4 + p_1\right)^2.$$

Here E is the total center-of-mass (CM) energy, q is the "momentum transfer," and one finds $s + t + u = 4m^2$. If we then define the reduced transition matrix element by

$$S = 1 + iT(s,t)(2\pi)^D\delta^D\left(\sum p\right) \tag{5.23}$$

and take the limit of large $s = E^2$, we find the high-energy approximation of the Born amplitude T_0 :

$$T_0(s,t) \simeq -8\pi G_D s^2/t.$$

5.1.4 Canonical approach and the S-Matrix

5.1.4.1 Asymptotic States: Quantization of Gauge Field

In this section we quantize the free volume-preserving diffeomorphism group gauge field. Solving the linearized field equations we express all: the fields, the inertial energy-momentum and the inner momentum constructed in section 5.1.2 in terms of creation and annihilation operators and appropriate polarization vectors. The field quanta carry both inertial energy-momentum and inner momentum. We then construct the gauge field Fock space and the propagator. Finally we establish the "gravitational limit" to connect the field quanta with observable gauge particles. Let us start with the Lagrangian density Eqn.(5.16) for the gauge field defined on $\mathbf{M}^4 \times \mathbf{M}^4$

$$\begin{aligned}\mathcal{L}_G\left(A_\mu{}^\alpha, \partial^\nu A_\mu{}^\alpha; \nabla_\beta A_\mu{}^\alpha\right) &= \frac{1}{4\Lambda^2} F_{\mu\nu}{}^\alpha(x,X)\cdot F^{\mu\nu}{}_\alpha(x,X) \\ &+ \frac{\lambda}{2\Lambda^2}\partial_\mu A^\mu{}_\alpha(x,X)\cdot\partial^\nu A_\nu{}^\alpha(x,X) - \frac{\mu^2}{2\Lambda^2} A^\mu{}_\alpha(x,X)\cdot A_\mu{}^\alpha(x,X)\end{aligned} \tag{5.24}$$

adding both a gauge-fixing and a mass term to be able to canonically quantize and to deal with eventual infrared problems. The Euler-Lagrange equation for the gauge field is

$$\left(-\partial^2 - \mu^2\right) A^\mu_\alpha(x,X) + (1-\lambda)\partial^\mu\left(\partial_\rho A^\rho{}_\alpha(x,X)\right) = J^\mu{}_\alpha(x,X), \tag{5.25}$$

where both gauge field self-interactions and interactions with matter currents have been collected in the current $J_\mu{}^\alpha$ which by construction is divergence-free in space-time as well as in inner space

$$\partial^\mu J_\mu{}^\alpha(x,X) = 0, \quad \nabla_\alpha J_\mu{}^\alpha(x,X) = 0. \tag{5.26}$$

Taking the space-time divergence of Eqn.(5.25)

$$\left(-\partial^2 - \frac{\mu^2}{\lambda}\right)\left(\partial_\rho A^\rho_\alpha(x,X)\right) = 0$$

we find that with or without interactions present the divergence of the gauge field $\partial_\rho A^\rho{}_\alpha$ is a free scalar field with mass $\frac{\mu^2}{\lambda}$. This in turn allows us to define the transversal part

of the gauge field as usual

$$A_\mu^{T\alpha}(x,X) = A_\mu{}^\alpha(x,X) + \frac{\lambda}{\mu^2}\partial_\mu\left(\partial^\rho A_\rho{}^\alpha(x,X)\right), \partial^\mu A_\mu^{T\alpha}(x,X) = 0 \tag{5.27}$$

To keep calculations simple we set the gauge parameter

$$\lambda = 1$$

in the rest of the section. With this choice of λ and with or without interactions present the transversal part of the gauge field fulfils

$$\left(-\partial^2 - \mu^2\right) A_\mu^{T\alpha}(x,X) = J_\mu{}^\alpha(x,X). \tag{5.28}$$

To canonically quantize we first calculate the canonically conjugate field momenta

$$\begin{aligned}\Pi^\nu{}_\beta(x,X) &= \frac{\partial \mathcal{L}_G}{\partial\left(\partial^0 A_\nu{}^\beta(x,X)\right)} \\ &= \Lambda^{-2} F_0{}^\nu{}_\beta(x,X) + \Lambda^{-2}\eta_0{}^\nu \partial_\rho A^\rho{}_\beta(x,X)\end{aligned} \tag{5.29}$$

which live in the gauge algebra like the gauge fields

$$\nabla_\alpha A_\mu{}^\alpha(x,X) = 0, \quad \nabla^\beta \Pi^\nu{}_\beta(x,X) = 0 \tag{5.30}$$

Defining the delta function transversal in inner space

$$\delta^T_{\alpha\beta}(X-Y) = \int \frac{d^4K}{(2\pi)^4}\Lambda^4 e^{-iK(X-Y)}\left(\eta_{\alpha\beta} - \frac{K_\alpha K_\beta}{K^2}\right) \tag{5.31}$$

we next impose generalized canonical equal-time commutation relations

$$\begin{aligned}&\left[A_\mu{}^\alpha(t,\underline{x};X), A^\nu{}_\beta(t,\underline{y};Y)\right] = 0 \\ &\left[\Pi_\mu{}^\alpha(t,\underline{x};X), I^\nu{}_\beta(t,\underline{y};Y)\right] = 0 \\ &\left[A_\mu{}^\alpha(t,\underline{x};X), II^\nu_\beta(t,\underline{y};Y)\right] = i\eta_\mu{}^{\nu T}\delta^\alpha{}_\beta(X-Y)\delta^3(\underline{x}-\underline{y})\end{aligned} \tag{5.32}$$

consistent with the conditions Eqns.(5.30) on the gauge fields and their conjugate momenta.

It is straightforward to re-express the canonical commutation relations Eqns.(5.32) in terms of the gauge fields and their first time derivative

$$\begin{aligned}
&\left[A_\mu{}^\alpha(t,\underline{x};X), A^\nu{}_\beta(t,\underline{y};Y)\right] = 0 \\
&\left[\dot{A}_\mu{}^\alpha(t,\underline{x};X), \dot{A}_{\beta\beta}(t,\underline{y};Y)\right] = 0 \\
&\left[A_\mu{}^\alpha(t,\underline{x};X), \dot{A}^\nu_\beta(t,\underline{y};Y)\right] = i\eta_\mu{}^\nu \Lambda^{2T}\delta^\alpha{}_\beta(X-Y)\delta^3(\underline{x}-\underline{y})
\end{aligned} \tag{5.33}$$

indicating that the sixteen $A_\mu{}^\alpha$ are quantized like a set of scalar fields. Some, however, will have negative norm in Hilbert space, a fact we will have to deal with below to arrive at a sensible theory.

Next we "solve" the field equation Eqn. (5.25) and the constraint Eqn.(5.26) for $\lambda = 1$ by Fourier transforming

$$\begin{aligned}
A_\rho{}^\alpha(x,X) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \int \frac{d^4K}{(2\pi)^4}\Lambda^4 \sum_{\gamma=0}^{3}\sum_{\Gamma=1}^{3} \\
\varepsilon_\rho(k,\gamma)\mathcal{E}^\alpha(K,\Gamma)\left\{a_+(\underline{k},\gamma;K,\Gamma)e^{-ikx-iKX} + \text{ h.c. }\right\}
\end{aligned} \tag{5.34}$$

and putting k^μ on the mass shell

$$k^2 = \mu^2 \quad \text{or} \quad \omega_k = \sqrt{\underline{k}^2+\mu^2}. \tag{5.35}$$

Above $\gamma = 0,1,2,3$ and $\Gamma = 1,2,3$ denote the polarization degrees of freedom,

$$\varepsilon_\rho(k,0) = \frac{k_\rho}{\mu} \quad \text{and} \quad \varepsilon_\rho(k,\gamma), \quad \gamma = 1,2,3 \tag{5.36}$$

and

$$\mathcal{E}^\alpha(K,\Gamma), \quad \Gamma = 1,2,3 \tag{5.37}$$

the corresponding polarization vectors in space-time and inner space. Note that $\Gamma = 0$ does not appear due to the transversality $\nabla_\alpha A_\mu{}^\alpha(x,X) = 0$ of the gauge field in inner

space. ε_ρ and $\mathcal{E}^\alpha$ obey the following relations

$$k^\rho \cdot \varepsilon_\rho(k,\gamma \neq 0) = 0, \quad \varepsilon_\rho(k,\gamma) \cdot \varepsilon^\rho(k,\gamma') = \eta^{\gamma\gamma'}$$
$$\sum_{\gamma=1}^{3} \varepsilon^\rho(k,\gamma)\varepsilon^\sigma(k,\gamma) = -\eta^{\rho\sigma} + \frac{k^\rho k^\sigma}{\mu^2}$$

$$K_\alpha \cdot \mathcal{E}^\alpha(K,\Gamma) = 0, \quad \mathcal{E}^\alpha(K,\Gamma) \cdot \mathcal{E}_\alpha(K,\Gamma') = \eta^{\Gamma\Gamma'}$$
$$\sum_{\Gamma=1}^{3} \mathcal{E}_\alpha(K,\Gamma)\mathcal{E}_\beta(K,\Gamma) = -\eta_{\alpha\beta} + \frac{K_\alpha K_\beta}{K^2} \text{ for } K^2 \geq 0$$

To ensure positivity of the gauge field energy the support of the $a_+$is restricted to time- and light-like vectors in inner space

$$\text{supp}\left(a_+(\underline{k},\gamma;K,\Gamma)\right) = \mathbf{R}^3 \times \left(\mathbf{V}^+(K) \cup \mathbf{V}^-(K)\right).$$

Inversion yields for a_+

$$a_+(\underline{k},\gamma;K,\Gamma) = i\eta^{\gamma\gamma}\eta^{\Gamma\Gamma} \int d^3x \int d^4X \Lambda^{-4}$$
$$e^{ikx+iKX}\partial_0\left(\varepsilon^\rho(k,\gamma)\mathcal{E}_\alpha(K,\Gamma)A^\alpha_\rho(x,X)(t,\underline{x};X)\right)$$

with an analogous expression for $a_+^\dagger$. The commutation relations for the $a_+, a_+^\dagger$ are then easily obtained

$$[a_+(\underline{k},\gamma;K,\Gamma), a_+(\underline{h},\gamma';H,\Gamma')] = 0$$
$$\left[a_+^\dagger(\underline{k},\gamma;K,\Gamma), a_+^\dagger(\underline{h},\gamma';H,\Gamma')\right] = 0$$
$$\left[a_+(\underline{k},\gamma;K,\Gamma), a_+^\dagger(\underline{h},\gamma';H,\Gamma')\right] = 2\omega_k\eta^{\gamma\gamma'}\eta^{\Gamma\Gamma'}$$
$$\Lambda^{-2}(2\pi)^4\delta^4(K-H)(2\pi)^3\delta^3(\underline{k}-\underline{h})$$

and show that states have positive norm only for $\gamma,\gamma' = 1,2,3$. The canonical energy-

momentum tensor is calculated as usual

$$\begin{aligned}\Theta^{\mu\nu}(x) = \int d^4X\Lambda^{-6}\{&F^{\mu\rho}{}_{\alpha}(x,X)\cdot\partial^{\nu}A_{\rho}{}^{\alpha}(x,X)\\ &-\frac{1}{4}\eta^{\mu\nu}F_{\rho\sigma}{}^{\alpha}(x,X)\cdot F^{\rho\sigma}{}_{\alpha}(x,X)\\ &+\partial_{\rho}A^{\rho}{}_{\alpha}(x,X)\cdot\partial^{\nu}A^{\mu\alpha}(x,X)\\ &-\frac{1}{2}\eta^{\mu\nu}\partial_{\rho}A^{\rho}{}_{\alpha}(x,X)\cdot\partial^{\sigma}A_{\sigma}{}^{\alpha}(x,X)\\ &-\frac{\mu^2}{2}\eta^{\mu\nu}A^{\rho}_{\alpha}(x,X)\cdot A_{\rho}{}^{\alpha}(x,X)\Big\}\end{aligned}$$

Next we re-express both the momentum three vector

$$\mathbf{p}^{i} = \int d^3x\int d^4X\Lambda^{-6}\partial^0 A^{\rho}_{\alpha}(x,X)\cdot\partial^{i}A_{\rho}{}^{\alpha}(x,X)$$

Next we re-express both the momentum three vector

$$\mathbf{p}^{i} = \int d^3x\int d^4X\Lambda^{-6}\partial^0 A^{\rho}{}_{\alpha}(x,X)\cdot\partial^{i}A_{\rho}{}^{\alpha}(x,X)$$

and the energy

$$\begin{aligned}\mathbf{p}^{0} = \frac{1}{2}\int d^3x\int d^4XA^{-4}\big\{&\partial^0 A^{\rho}{}_{\alpha}(x,X)\cdot\partial^0 A_{\rho}{}^{\alpha}(x,X)\\ &+\partial^{i}A^{\rho}{}_{\alpha}(x,X)\cdot\partial^{i}A_{\rho}{}^{\alpha}(x,X)+\mu^2A^{\rho}{}_{\alpha}(x,X)\cdot A_{\rho}{}^{\alpha}(x,X)\big\}\end{aligned}$$

in terms of the $a_{+},a^{\dagger}_{+}$ obtaining the covariant inertial energy-momentum vector

$$\begin{aligned}\mathbf{p}^{\nu} = \frac{1}{2}\int\frac{d^3k}{(2\pi)^3 2\omega_k}\int\frac{d^4K}{(2\pi)^4}\Lambda^2k^{\nu}\sum_{\gamma=0}^{3}\sum_{\Gamma=1}^{3}\\ \eta^{\gamma\gamma}\eta^{\Gamma\Gamma}\Big\{a_{+}(\underline{k},\gamma;K,\Gamma)a^{\dagger}_{+}(\underline{k},\gamma;K,\Gamma)+\ \text{h.c.}\ \Big\}\end{aligned}$$

Note that the energy $\mathbf{p}^0>0$ is positive if the summation is extended over $\gamma=1,2,3$ only which is the case for purely transversal states.

In an analogous way we next determine the inner momentum tensor

$$J^{\mu}_{\beta}(x) = \int d^4X\Lambda^{-6}\left\{F^{\mu\rho}{}_{\alpha}(x,X)\cdot\nabla_{\beta}A_{\rho}{}^{\alpha}(x,X)\right.$$
$$\left.+\partial_{\rho}A^{\rho}{}_{\alpha}(x,X)\cdot\nabla_{\beta}A^{\mu\alpha}(x,X)\right\}$$

and the conserved inner momentum vector

$$\begin{aligned}\mathbf{P}_{\beta} =& \int d^3x\int d^4X\Lambda^{-6}\partial^0 A^{\rho}{}_{\alpha}(x,X)\cdot\nabla_{\beta}A_{\rho}{}^{\alpha}(x,X)\\ =&\frac{1}{2}\int\frac{d^3k}{(2\pi)^3 2\omega_k}\int\frac{d^4K}{(2\pi)^4}\Lambda^2 K_{\beta}\sum_{\gamma=0}^{3}\sum_{\Gamma=1}^{3}\\ &\eta^{\gamma\gamma}\eta^{\Gamma\Gamma}\left\{a_{+}(\underline{k},\gamma;K,\Gamma)a^{\dagger}_{+}(\underline{k},\gamma;K,\Gamma)+\ \text{h.c.}\ \right\}.\end{aligned}$$

All of the above formula are correct again up to the introduction of normal ordering.

The calculation of the commutators of the inertial energy-momentum and the inner momentum with $a^{\dagger}_{+}$ yields

$$\left[\mathbf{p}_{\mu},a^{\dagger}_{+}(\underline{k},\gamma;K,\Gamma)\right]=\eta^{\gamma\gamma}\eta^{\Gamma\Gamma}k_{\mu}a^{\dagger}_{+}(\underline{k},\gamma;K,\Gamma)$$
$$\left[\mathbf{P}_{\alpha},a^{\dagger}_{+}(\underline{k},\gamma;K,\Gamma)\right]=\eta^{\gamma\gamma}\eta^{\Gamma\Gamma}K_{\alpha}a^{\dagger}_{+}(\underline{k},\gamma;K,\Gamma)$$

allowing for an easy cross-check of the conservation of both types of momenta

$$[\mathbf{H},\mathbf{p}_{\mu}]=0,\quad[\mathbf{H},\mathbf{P}_{\alpha}]=0$$

We establish the usual particle interpretation starting with a vacuum state $|0\rangle$ with $\langle 0\mid 0\rangle=1$ which is annihilated by the destruction operator a_{+}

$$a_{+}(\underline{k},\gamma;K,\Gamma)|0\rangle=0$$

and out of which the creation operator $a^{\dagger}_{+}$ generates one-particle states

$$a^{\dagger}_{+}(\underline{k},\gamma;K,\Gamma)|0\rangle=\ \text{one-particle state}$$

with definite energy-momentum k, inner momentum K and polarizations γ,Γ and with

normalization

$$\left\langle 0 \left| a_+ \left(\underline{h}, \gamma'; H, \Gamma'\right) a_+^\dagger(\underline{k}, \gamma; K, \Gamma) \right| 0 \right\rangle = 2\omega_k \eta^{\gamma\gamma'} \eta^{\Gamma\Gamma'}$$
$$\Lambda^{-2}(2\pi)^4 \delta^4(K-H)(2\pi)^3 \delta^3(\underline{k}-\underline{h}).$$

Acting on a simultaneous eigenstate $|h, H\rangle$ of $\mathbf{p}_\mu$ and $\mathbf{P}_\alpha$ with eigenvalues h_μ and H_α respectively we find

$$\mathbf{p}_\mu a_+^\dagger(\underline{k}, \gamma; K, \Gamma)|h, H\rangle = \eta^{\gamma\gamma}\eta^{\Gamma\Gamma}\left(h_\mu + k_\mu\right) a_+^\dagger(\underline{k}, \gamma; K, \Gamma)|h, H\rangle$$
$$\mathbf{p}_\mu a_+(\underline{k}, \gamma; K, \Gamma)|h, H\rangle = \eta^{\gamma\gamma}\eta^{\Gamma\Gamma}\left(h_\mu - k_\mu\right) a_+(\underline{k}, \gamma; K, \Gamma)|h, H\rangle$$
$$\mathbf{P}_\alpha a_+^\dagger(\underline{k}, \gamma; K, \Gamma)|h, H\rangle = \eta^{\gamma\gamma}\eta^{\Gamma\Gamma}\left(H_\alpha + K_\alpha\right) a_+^\dagger(\underline{k}, \gamma; K, \Gamma)|h, H\rangle$$
$$\mathbf{P}_\alpha a_+(\underline{k}, \gamma; K, \Gamma)|h, H\rangle = \eta^{\gamma\gamma}\eta^{\Gamma\Gamma}\left(H_\alpha - K_\alpha\right) a_+(\underline{k}, \gamma; K, \Gamma)|h, H\rangle$$

which allows us to construct the Fock space of stationary states by applying multiple creation operators on the vacuum state, however, at the price of having to deal with an indefinite metric at this point as is usual in the Stueckelberg-Gupta-Bleuler approach for quantizing gauge fields. Finally we calculate the time-ordered product of two field operators to obtain the Feynman propagator for free gauge fields

$$\left\langle 0 \left| T\left(A_\mu{}^\alpha(x, X) A_\nu{}^\beta(x, X)\right) \right| 0 \right\rangle = -i\Lambda^2 T^{\alpha\beta}(X-Y).$$
$$\int \frac{d^4k}{(2\pi)^4} e^{-ik(x-y)} \frac{\eta_{\mu\nu}}{k^2 - \mu^2 + i\varepsilon}$$

which is local in inner space. Before turning to discuss the "gravitational limit" we define the Fock sub-space of positive norm states requiring their annihilation by $\partial^\rho A_\rho^{(-)\alpha}$

$$\mathcal{F}_P = \left\{ |\alpha\rangle \left| \partial^\rho A_\rho^{(-)\alpha}(x, X) \right| \alpha \right\rangle = 0 \right\},$$

where $A_\rho^{(-)\alpha}$ is given by

$$A_\rho^{(-)\alpha}(x, X) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \int \frac{d^4K}{(2\pi)^4} \Lambda^4 \sum_{\gamma=0}^{3} \sum_{\Gamma=1}^{3}$$
$$\varepsilon_\rho(k, \gamma) \mathcal{E}^\alpha(K, \Gamma) a_+(\underline{k}, \gamma; K, \Gamma) e^{-ikx - iKX}$$

and its divergence by

$$\partial^\rho A_\rho^{(-)\alpha}(x,X) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \int \frac{d^4K}{(2\pi)^4} \Lambda^4 \sum_{\Gamma=0}^{3} \mu$$
$$\mathcal{E}^\alpha(K,\Gamma) a_+(\underline{k},0;K,\Gamma) e^{-ikx-iKX}$$

containing only the destruction operators $a_+$for $\gamma = 0$. Due to Eqn.(101) $\mathcal{F}_P$ contains positive norm states only

$$a_+^\dagger(\underline{k},\gamma;K,\Gamma)|0\rangle = \text{ positive norm states for } \gamma,\Gamma = 1,2,3$$

as required for a consistent probabilistic interpretation of the theory. Finally we introduce the "gravitational limit" by mapping K onto k

$$\bar{a}^\dagger(\underline{k},\gamma,\Gamma) = \lim_{K\to k} a_+^\dagger(\underline{k},\gamma;K,\Gamma).$$

The normalization of these states involves again a regularization of the inner volume

$$\begin{aligned}\left[\bar{a}(\underline{k},\gamma,\Gamma), \bar{a}^\dagger(\underline{h},\gamma',\Gamma')\right] = \lim_{K\to k}\lim_{H\to h} 2\omega_k \eta^{\gamma\gamma'}\eta^{\Gamma\Gamma'} \\ = \Lambda^{-2}(2\pi)^4\delta^4(K-H)(2\pi)^3\delta^3(\underline{k}-\underline{h}) \\ = 2\omega_k\eta^{\gamma\gamma'}\eta^{\Gamma\Gamma'}\frac{V'}{\Lambda^4}\Lambda^2(2\pi)^3\delta^3(\underline{k}-\underline{h}) \\ = 2\omega_k\eta^{\gamma\gamma'}\eta^{\Gamma\Gamma'}\Lambda^2(2\pi)^3\delta^3(\underline{k}-\underline{h})\end{aligned}$$

and yields properly normalized destruction and creation operators belonging to a free gauge field (but with field quanta still remembering that they carry both inertial and inner energy-momentum).

The physical Fock space $\mathcal{F}_{\text{phys}}$ of positive norm states is again obtained requiring their annihilation by $\partial^\rho \bar{A}_\rho^{(-)\alpha}$

$$\mathcal{F}_{\text{phys}} = \left\{|\beta\rangle \left|\partial^\rho \bar{A}_\rho^{(-)\alpha}(x)\right| \beta\right\rangle = 0\Big\},$$

where

$$\bar{A}_\rho^{(-)\alpha}(x) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \sum_{\gamma=0}^{3}\sum_{\Gamma=1}^{3} \varepsilon_\rho(k,\gamma)\mathcal{E}^\alpha(k,\Gamma)\bar{a}(\underline{k},\gamma,\Gamma)e^{-ikx}$$

and

$$\partial^\rho \bar{A}^{(-)\alpha}_\rho(x) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \mu \sum_{\Gamma=1}^{3} \mathcal{E}^\alpha(k,\Gamma)\bar{a}(\underline{k},0,\Gamma)e^{-ikx}$$

The positive norm one-particle states

$$\bar{a}^\dagger(\underline{k},\gamma,\Gamma)|0\rangle = \text{ physical states for } \gamma,\Gamma = 1,2,3$$

represent then the asymptotic field quanta which correspond to the observable gravitons in our approach.

5.1.4.2 S-Matrix

In this section we first introduce the operator **S** mapping the asymptotic in-Fock space onto the asymptotic out-Fock space and discuss its properties. We then define the S-matrix S in quantum gravity as the gravitational limit of the operator **S** mapping the physical *in*-Fock space onto the physical out-Fock space. S is shown to be a unitary operator on the asymptotic physical Fock space if **S** is on the asymptotic Fock space. Let us define the operator **S** by its matrix elements

$$\mathrm{S}_{h_j,H_j;k_i,K_i} \equiv \langle h_1,H_1;\ldots;h_m,H_m \text{ out } | \, k_1,K_1;\ldots;k_n,K_n \text{ in } \rangle$$

or

$$\mathbf{S}_{h_j,H_j;k_i,K_i} = \langle h_1,H_1;\ldots;h_m,H_m \text{ in } |\mathbf{S}| k_1,K_1;\ldots;k_n,K_n \text{ in } \rangle$$

Note that we subsume all quantum numbers other than k and K characterizing an asymptotic stationary state in the above notation as they add no new features in our context.

S maps the asymptotic *in*-Fock space $\mathcal{F}_{\text{in}}$ onto the asymptotic out-Fock space $\mathcal{F}_{\text{out}}$

$$\langle h_1,H_1;\ldots;h_m,H_m \text{ in } | \, \mathbf{S} = \langle h_1,H_1;\ldots;h_m,H_m \text{ out } |$$

and is invertible by construction

$$\langle h_1,H_1;\ldots;h_m,H_m \text{ out } | \, \mathbf{S}^{-1} = \langle h_1,H_1;\ldots;h_m,H_m \text{ in } |$$

Next we list a few of the key properties of **S** :

A) Invariance of the vacuum yields

$$\langle 0 \text{ in } |\mathbf{S} = \langle 0 \text{ out } | = e^{i\alpha}\langle 0 \text{ in } |$$

and its uniqueness allows us to set the phase equal to zero so that

$$\langle 0 \text{ out } | = \langle 0 \text{ in } | = \langle 0|.$$

B) Invariance of the one-particle states yields

$$\begin{aligned}\langle p, P \text{ in } |\mathbf{S}|p, P \text{ in } \rangle &= \langle p, P \text{ out } |p, P \text{ in } \rangle \\ &= \langle p, P \text{ in } |p, P \text{ in } \rangle = 1\end{aligned}$$

as we have

$$| \, p, P \text{ in } \rangle = | \, p, P \text{ out } \rangle = |p, P\rangle$$

C) The operator adjoint to $\mathbf{S}$ is defined by

$$\mathbf{S}^\dagger \mid k_1, K_1; \ldots; k_n, K_n \text{ in } \big\rangle = \mid k_1, K_1; \ldots; k_n, K_n \text{ out } \big\rangle$$

and $\mathbf{S}$ is by construction unitary

$$\begin{aligned}&\big\langle h_1, H_1; \ldots; h_m, H_m \text{ in } \big|\mathbf{S}\mathbf{S}^\dagger\big| \, k_1, K_1; \ldots; k_n, K_n \text{ in } \big\rangle \\ &\quad = \langle h_1, H_1; \ldots; h_m, H_m \text{ out } | \, k_1, K_1; \ldots; k_n, K_n \text{ out } \rangle \\ &\quad = \delta_{h_j, H_j; k_i, K_i}\end{aligned}$$

or

$$\mathbf{S}\mathbf{S}^\dagger = \mathbf{S}^\dagger\mathbf{S} = \mathbf{1}$$

if the sets of ortho-normal vectors spanning the asymptotic in- and outFock spaces

$$| \, k_1, K_1; \ldots; k_n, K_n \text{ in } \rangle \, , \quad | \, k_1, K_1; \ldots; k_n, K_n \text{ out } \rangle$$

in Eqn. (123) are complete. Note that in the case of gauge fields $\mathbf{S}$ is pseudo-unitary only and its unitarity on the asymptotic *in* - and out-Fock subspaces of positive norm states has to be proven. In the case of the gauge field $A_\mu{}^\alpha(x, X)$ we have established that proof in [10].

Next we define the S-matrix S in quantum gravity by the gravitational limit of the

matrix elements of the operator $\mathbf{S}$

$$\begin{aligned} S_{h_j,k_i} &\equiv \lim_{H_j\to h_j}\lim_{K_i\to k_i}\mathbf{S}_{h_j,H_j;k_i,K_i} \\ &= \lim_{H_j\to h_j}\lim_{K_i\to k_i}\langle h_1,H_1;\ldots;h_m,H_m \text{ out } | \, k_1,K_1;\ldots;k_n,K_n \text{ in } \Big\rangle \\ &= \langle h_1\ldots h_m \text{ out } | \, k_1\ldots k_n \text{ in } \rangle \\ &= \langle h_1\ldots h_m \text{ in } | S | k_1\ldots k_n \text{ in } \rangle \end{aligned}$$

The operator S maps the asymptotic physical in-Fock space onto the asymptotic physical out-Fock space

$$\langle h_1\ldots h_m \text{ in } | \, S = \langle h_1\ldots h_m \text{ out } |$$

and is invertible

$$\langle h_1\ldots h_m \text{ out } | \, S^{-1} = \langle h_1\ldots h_m \text{ in } |$$

The properties A), B) and C) hold again: A') Eqn.(118) yields

$$\langle 0 \text{ in } | S = \langle 0 \text{ out } | = e^{i\beta}\langle 0 \text{ in } |$$

23 and we can again set the phase equal to zero so that

$$\langle 0 \text{ out } | = \langle 0 \text{ in } | = \langle 0|.$$

B') Eqn.(120) yields

$$\begin{aligned} \langle p \text{ in } | S | p \text{ in } \rangle &= \langle p \text{ out } | p \text{ in } \rangle \\ &= \langle p \text{ in } | p \text{ in } \rangle = 1 \end{aligned}$$

as we have again

$$| \, p \text{ in } \rangle = | \, p \text{ out } \rangle = |p\rangle.$$

C') To prove the unitarity of S on the asymptotic physical Fock space we introduce the self-adjoint projection operator $\mathbf{P} = \mathbf{P}^2$ which maps any in- or out-state in the asymptotic positive-norm Fock space on its gravitational-limit state vector in the asymptotic physical Fock space $\mathcal{F}_{\text{phys}}$

$$\mathbf{P} \mid k_1,K_1;\ldots;k_n,K_n \text{ in } \rangle = \lim_{K_i\to k_i} \mid k_1,K_1;\ldots;k_n,K_n \text{ in } \Big\rangle .$$

Note that $\mathbf{P}$ is the identity in the asymptotic physical Fock space

$$\mathbf{P} = \mathbf{1}_{\text{phys}} .$$

We can now express S in terms of $\mathbf{S}$ and $\mathbf{P}$ as

$$\langle \dots \text{ in } | \mathbf{P} S = \langle \dots \text{ in } | \mathbf{SP}.$$

Assuming S to be unitary allows us to write

$$\begin{aligned} \mathbf{1}_{\text{phys}} &= \mathbf{P}1\mathbf{P} = \mathbf{P}\mathbf{S}^\dagger\mathbf{S}\mathbf{P} \\ &= S^\dagger \mathbf{P}\mathbf{P} S = S^\dagger S \end{aligned}$$

This proves the unitarity of the gravitational S-matrix S if $\mathbf{S}$ is unitary which is a key pre-requisite for a viable physical theory.

5.1.5 Path Integral Approach to Quantum Gravity

The basic idea of the Feynman path integral is that the amplitude to go from a state with metric g_1, and matter fields ϕ_1 at time t_1 to a state with metric g_2 and matter fields ϕ_2 at time t_2 is given by an integral over all field configurations which take the given values at times t_1 and t_2 :

$$\langle g_2, \phi_2, t_2 \mid g_1, \phi_1, t_1 \rangle = \int D[g] D[\phi] \exp(iI[g, \phi]) \tag{5.38}$$

where $D[g]$ is a measure on the space of all metrics, $D[\phi]$ is a measure on the space of all matter fields, I is the action, and the integral is taken over all field configurations with the given initial and final values. (we are using units in which $c = \hbar = k = 1$.) The gravitational contribution to the action is normally taken to be

$$\frac{1}{16\pi G} \int R(-g)^{1/2} d^4x \tag{5.39}$$

However, the Ricci scalar R contains second derivatives of the metric. In order to obtain an action which depends only on first derivatives, as is required by the path-

integral method, one has to remove the second derivatives by integrating by parts. This produces a surface term which can be written in the form

$$\frac{1}{8\pi G}\int K(h)^{1/2}d^3x + C$$

where the integral is taken over the boundary of the region for which the action is being evaluated, K is the trace of the second fundamental form of the boundary in the metric g, h is the induced metric on the boundary, and C is a term which depends only on the boundary and not on the particular metric g.In order to make sure that one registers this surface term correctly one has to join the initial and final spacelike surfaces by a timelike tube at some large radius r_0. It is convenient to rotate the time interval on this timelike tube between the two surfaces into the complex plane so that it becomes purely imaginary. This makes the metric on the boundary positive definite so that the path integral can be taken over all positive-definite metrics g that induce the given metric for the boundary. Suppose that one wants to find the number $n(E)dE$ of states of the gravitational and matter fields which have energy between E and $E + dE$ as measured from infinity. This will be given by

$$n = \frac{1}{2\pi i}\int_{-i_\infty}^{i_\infty} Z(\beta)\exp(\beta E)d\beta \tag{5.40}$$

where

$$Z(\beta) = \sum_n \langle g_n, \phi_n|\exp(-\beta H)|g_n, \phi_n\rangle \tag{5.41}$$

is the partition function for the system consisting of the gravitational and matter fields contained in a box of radius r_0 at a temperature $T = \beta^{-1}$. This partition function can be expressed as a path integral over all matter and gravitational fields that are periodic in imaginary time with period β, i.e.,

$$Z = \int D[g]D[\phi]\exp(-\hat{I}) \tag{5.42}$$

where $\hat{I} = -iI$ is the Euclidean action and the path integral is taken over all positive-definite metrics g whose boundary is a two sphere of radius r_0 times a circle of circumference β representing the periodically identified imaginary time axis. One would expect that the dominant contribution in the path integral for Z would come from

metrics g and matter fields ϕ that are near background fields g_0, ϕ_0 that extremize the action, i.e., are solutions of the classical field equations with the given periodicity and boundary conditions. Neglecting, for the moment, the question of the radius of convergence, one can expand the action in a Taylor series about the background fields $\hat{I}[g,\phi] = \hat{I}\,[g_0,\phi_0] + I_2[\tilde{g},\tilde{\phi}]+$ higher-order terms where $g = g_0 + \tilde{g}, \phi = \phi_0 + \tilde{\phi}$, and I_2 is quadratic in the perturbations $\tilde{g}$ and $\tilde{\phi}$. If one neglects the higher-order terms, then

$$\ln Z = -\hat{I}\,[g_0,\phi_0] + \ln \int D[g,\phi] \exp\left(-I_2[\tilde{g},\tilde{\phi}]\right) \tag{5.43}$$

One can regard the first term in the equation above as the contribution of the background field to the partition function and the second term as the contribution of thermal gravitons and matter quanta the background geometry.

5.2 Path Integrals and Introductory String Theory

5.2.1 Sum over worldsheets and The Polyakov path integral

The Feynman path integral is a natural approach to describe interactions in string theory and one way to express a quantum theory. Amplitudes are calculated by summing all possible histories and interpolating between the start and end states in route integral quantization. Each piece of history is given a certain amount of weight.

$$\exp\left(iS_{\mathrm{cl}}/\hbar\right) \tag{5.44}$$

with S_{cl} For the given history, the classical action. As seen in figure 5.1(a)for the open string and figure 5.1(b) for the closed string, an amplitude is defined in string theory by summing over all world-sheets linking specified beginning and end curves. The free propagator is produced by adding the equivalent sums for relativistic point particles.

Strings can interact in a variety of ways, as might be imagined. One example is a contact interaction, which occurs when two strings cross. A long-range force mediated by a quantum field is another possibility. However, such interactions cannot be added to string theory in a fashion that is compatible with the symmetries; we shall see why

this is true later. Instead, only interactions that are already implied in the total over world-sheets are permitted. Take, for instance, the world-sheets depicted in Figure 5.2. Figure 5.2(a) appears to be a quantum correction to figure 5.1(a)'s string amplitude, involving intermediate states with two open strings. There are three external variables in figure 5.2(b)

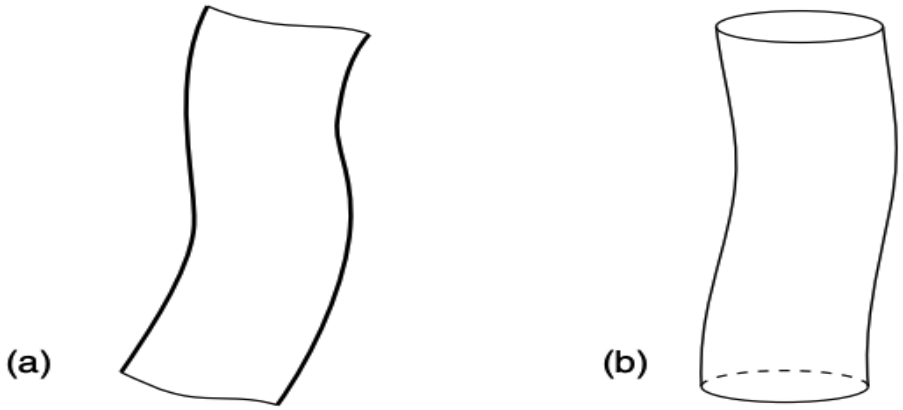

Figure 5.1: (a) An open string world-sheet with the topology of a strip. The heavier curves are the world-lines of string endpoints. (b) A closed string world-sheet with the topology of a cylinder.

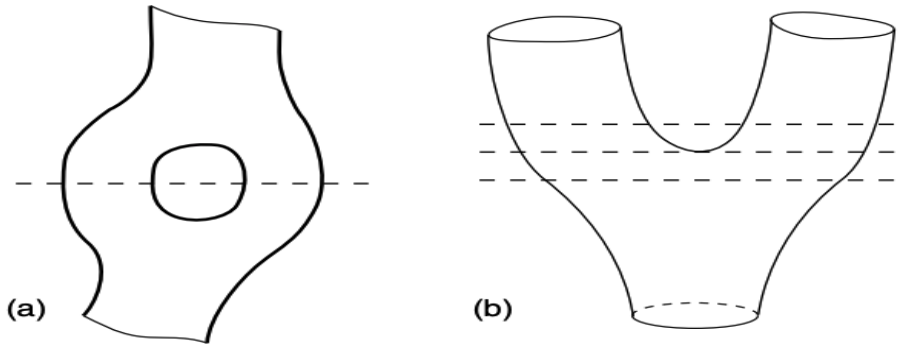

Figure 5.2: (a) Quantum correction to open string propagation. (b) Decay of one closed string into two. The dashed lines are time-slice.

closed strings and represents one string decaying into two, it turns out, is the proper method for introducing interactions into string theory. We'll show how these interactions result in a finite and unitary theory that incorporates gravity. Consider the procedure depicted in figure 5.2(b) as observed at different periods. A closed string breaks into two, or two strings come together in the reverse procedure. This is the

fundamental interaction between closed strings. All particles are produced as various states of excitation of the string in closed string theory, and all interactions (gauge, gravitational, etc.) are obtained as various states of excitation of the string.

Polyakov Path Integral

We now begin to develop the sum over world-sheets, integrating over the fields of the Polyakov formalism. We make one change from the Minkowskian world-sheet metric γ_{ab} is replaced with a Euclidean worldsheet metric $g_{ab}(\sigma^1, \sigma^2)$, of signature $(+,+)$. The integral runs over all Euclidean metrics and over all embeddings $X^\mu(\sigma^1, \sigma^2)$ of the world-sheet in Minkowski spacetime:

$$\int [dX dg] \exp(-S)$$

The Euclidean action is

$$S = S_X + \lambda\chi$$

with

$$\begin{aligned} S_X &= \frac{1}{4\pi\alpha'} \int_M d^2\sigma g^{1/2} g^{ab} \partial_a X^\mu \partial_b X_\mu \\ \chi &= \frac{1}{4\pi} \int_M d^2\sigma g^{1/2} R + \frac{1}{2\pi} \int_{\partial M} dsk \end{aligned} \tag{5.45}$$

The geodesic curvature is denoted by k note that the boundary now is always spacelike. The advantage of the Euclidean path integral is that the integral over metrics is better defined. The topologically nontrivial world-sheets we have been describing can have nonsingular Euclidean metrics but not Minkowskian ones. We will take the Euclidean theory as our starting point, and we will show how to give it a precise definition and that it defines a consistent spacetime theory with the advertised properties. However, let us give a brief formal argument that it is equivalent to the Minkowski theory with which we began.

We start again with the example of the point particle, where the path integral

$$\int [d\eta dX] \exp\left[\frac{i}{2} \int d\tau \left(\eta^{-1} \dot{X}^\mu \dot{X}_\mu - \eta m^2\right)\right]$$

is oscillatory. The path integral over η and X^μ is a product of ordinary integrals, and

so we can deform contours just as in ordinary integration. If we take

$$\eta(\tau) \to e^{-i\theta}\eta(\tau), \quad X^0(\tau) \to e^{-i\theta}X^0(\tau)$$

for infinitesimal θ, all terms in the exponent acquire a negative real part and so this acts as a convergence factor. Now we can perform a contour rotation in field space, all the way to $\eta = -ie, X^0 = -iX^D$. The integral becomes

$$\int [\mathrm{de}\, dX] \exp\left[-\frac{1}{2}\int d\tau \left(e^{-1}\sum_{\mu=1}^{D}\dot{X}^\mu \dot{X}^\mu + em^2\right)\right]$$

This is the Euclidean point-particle analog of the path integral (3.2.1). We have just made a contour rotation, so the Euclidean path integral gives the same amplitude as the Minkowski one.

5.2.2 Path Integrals of Super-symmetric String theory

Finding a coherent mathematical framework that unifies quantum field theory with general relativity is one of the most important concerns in theoretical physics today. While the other fundamental interactions, such as electromagnetic, weak, and strong interactions, are well characterised by local quantum field theories, gravity has eluded any coherent quantum mechanical explanation. At the moment, superstring theory is the most promising approach to solving this problem. String theory began as an S-matrix theory of hadrons , but it was subsequently revealed that its spectrum always contains a massless spin 2 particle, coupling in the same manner as the graviton does in general relativity . The bosonic string, which depicts particles with just integer spin, is the earliest model. Later, space-time fermions were included into fermionic string theory . However, both theories feature a tachyonic particle in their spectra. The GSO architecture was used to address this challenge, resulting in a string theory with a space-time supersymmetric particle spectrum. This superstring theory quickly established itself as a viable contender for a consistent quantum theory that includes gravity. String theorists commonly believe that what we now know about superstrings is merely a small portion of a much larger structure that has yet to be discovered. It is impossible to do any non-perturbative computations or even provide a specification of the theory's ground state in its current form. Superstring theory is still distant

from providing predictions that can be tested by experiments because to this poor understanding. So far, all hints about what superstring theory is have come from its perturbation expansion. String perturbation theory is expressed as an increase in the number of loops, much like conventional quantum field theory. Each term is defined as a sum over world surfaces with a fixed number of handles, which represent the trajectories of strings propagating across space-time . A two-dimensional supersymmetric quan1 turn field theory linked in a Weyl invariant way to two-dimensional supergravity describes the sum over world surfaces in superstring theory. The interaction of the two-dimensional quantum field theory with the surface geometry is finite dimensions due to this Weyl invariance. The surface's non-trivial variations are parametrized by a finite collection of coordinates known as superinoduli. Over this supermoduli space, string amplitudes are integrals . The representation of Feynman diagrams as sums over world lines is the point particle analogue of this description. The string represents the supermoduli.Supermoduli are a string generalisation of proper time variables that parametrize the length of world lines. A key distinction between strings and point particles is that, although point particle interactions have specific locations in space-time, string theory interactions are entirely topological; there are no interaction sites on a world.surface. Because of this discrepancy, it is predicted that, unlike in quantum field theory, the loop corrections for superstring scattering amplitudes will not undergo renormalization and will be finite. The geometry of the target space-time is given a priori in the path-integral formulation of string theory, and the strings themselves are thought of as a disturbance on this classical background. String theory should, in theory, be able to determine the space-time geometry, thus this is plainly an incomplete explanation. Nonetheless, it is an essential topic whether superstring scattering amplitudes can be described consistently, that is, without infinities, tadpoles, or any other form of anomaly, inside a given spacetime.

A string propagating through space-time sweeps out a two-dimensional surface. For bosonic strings the location of this world surface is described by d scalar ficlds $x^{\mu}(\xi_1, \xi_2)$, defined on a two-dimensional parameter space. Here we will consider only closed string theories, so the parameter space has the form of a cylinder. The superstring has in addition to the bosonic coordinates $x^{\mu}(\xi_1, \xi_2)$ also intcrnal spin- ning degrees of freedom, represented by d fermionic fields $\psi^{\mu}(\xi_1, \xi_2)$. The bosonic and fermionic coordinates together constitute a two-dimensional supersymmetric system. By introducing in addition a two-dimensional metric $g = g_{nb} d\xi^a d\xi^b$ and a gravitino field χ_a, the sum over

fermionic surfaces can be defined as the integral[6]

$$\sum_{\substack{\text{fermionic}\\ \text{surfaces}}} = \int [dg d\chi dx^\mu d\psi^\mu]\, e^{-S(g,\chi,x^\mu,\psi^\mu)}$$

where $S(g,\chi,x,\psi)$ is the action of the (x^μ,ψ^μ) -system coupled to two-dimensional supergravity [8]. This defiuition of the sum over fermionic surfaces is made invariant under reparametrizations and local supersymmetry transformations on the world sheet. As a consequence, the functional integral (1.1) has a large redundancy, which has to be removed by gauge fixing. We choose the so-called conformal gauge

$$g_{ab} = \rho\delta_{ab} \quad \chi_a = \gamma_a\zeta$$

In this gauge the action $S(g,\chi,x,\psi)$ has the following form:

$$S_{gf} = \int d^2z \left(\frac{1}{2}\partial_z x^\mu \partial_{\bar{z}} x_\mu + \psi^\mu \partial_{\bar{z}}\psi_\mu + \bar{\psi}^\mu \partial_z \bar{\psi}_\mu\right)$$

Here $(z,\bar{z}) = (\xi_1 + i\xi_2, \xi_1 - i\xi_2)$ are complex coordinate such that $g = \rho dz d\bar{z}$. 'The decoupling of the factors ρ and ζ from this action is a consequence of the super-Weyl invariance of $S(g,\chi,x,\psi)$[8]. This invariance persists at the qt antum level only in the critical dimension $d = 10$, [6]. This means that, for $d = 10$, the (x^μ,ψ^μ) quantum field theory only feels the conformal class of the metric and the gravitino. These conformal equivalence classes are called super-Riemann surfaces . We will limit our discussion here as the Construction of S-Matrix for any type of String Theory is beyond the scope of this thesis.

CHAPTER 6

Concluding Remarks and future theoretical aspects

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6.1 Conclusion

The aim of this work was to make a complete theoretical analysis of the S-Matrix, as we are aware that now a days Particle Physicists both experimentalists and Theoreists extensively look for new physics coming out of the particle accelerators, where we collide a bunch of different particles and observe the zoo of both new and old particles coming out of them. It is evident that in most of our collider experiments we have a initial state of particles and finally after collision we have a final state of particles, due to the very high energy scale and consequently very less time scale it is impossible to tell exactly what the particles are doing during the period of collision. As an observer we only get to see the final outcoming particles and initial particles that we accelerated.This is where the mathematical machinery of S-Matrix comes into play.Computation of S-Matrix requires only information about the Initial state of particles prepared in long past and final state of particles. We use the asymptotically free approximation and Put several condition on our S-Matrix such as Unitarity and Analiticity. These approximations and restrictions are enough to Compute the S-Matrix theoretically and study the Scattering and collison experiments.

This is why we developed the theoretical understanding of the S-Matrix in several different formulations, fields and contexts. Our discussion started with a very basic and brief comparisons of the two major formulations of modern QFT ie the Canonical

and Path integral formulation, this was done in order to provide a context as to where we will start studying the S-Matrix.

We then moved towards the study of previous works done by the likes of Dirac, Dyson, Weinberg, Schwinger,Tomonaga,etc where we studied the Canonical formulation of the S-Matrix.We discussed the S-Matrix as a limit of Time evolution operator and discussed its perturbative form also known as the Dyson series. We also studied the properties and symmetries of the S-Matrix and finally its Unitarity, Implications and Proof of Unitarity towards the end of the chapter.

We did a complete study of the Path Integral formulation, and discussed the construction of the Functional form of S-Matrix. AT last we dedicated a whole Chapter towards studying various formulations and approaches to the problem of Quantizing gravity and constructed the S-matrix of Quantum Gravity. Again this is important because S-Matrix, its properties and restrictions may turn out to be a guiding path towards a fully consistent theory of Quantum Gravity. We also did a brief study of Path Integrals in the Introductory String theory towards the end.

6.2 Future scope and S-Matrix bootsrap

The S-matrix bootstrap is a numerical method that can be used to determine or constrain the scattering amplitudes of particles in quantum field theory using simple principles. Over the past few decades, some physicists have tried to use this technique to study different physics theories and phenomena. Researchers at Tel Aviv University, École Polytechnique Fédérale de Lausanne (EPFL) and the Perimeter institute and ICTP-SAIFR have been developing the S-matrix bootstrap further and trying to apply it to different areas of physics. In a recent paper published in Physical Review Letters, the team tried to use it to investigate string theory, the renowned physics theory representing the fundamental components of the universe as one-dimensional (1D) 'strings', instead of point-like particles.

"The S-matrix bootstrap is an old idea that was popular in the 60s but lost popularity with the emergence of quantum chromodynamics to describe the strong nuclear force," Andrea Guerrieri, one of the researchers who carried out the study, told Phys.org. "The goal of the S-matrix bootstrap is to determine (or constrain) the scattering amplitudes

of particles in quantum field theory using just basic principles, such as causality, special relativity and the fact that probabilities cannot be larger than 1. The novelty we brought to the topic was the proposal of a systematic numerical algorithm to implement all these principles."

While there are now a few dozens of past papers exploring physical systems using different versions of the S-matrix bootstrap, most of these works focus on massive particles. Guerrieri and his colleagues, however, were recently also able to use it to study scattering of massless particles, such as transverse fluctuations of a color flux tube in quantum chromodynamics or in massless pions.

"Once they realized that the method works for massless particles, they tried it for gravitons, which are the mediators of the gravitational force,"Subsequently, they chose to impose supersymmetry in 10 spacetime dimensions to reduce the technical hurdles of the problem."

The recent work carried out by Guerrieri, Penedones and their colleague Pedro Vieira applies to any theory of quantum gravity. In their study, however, they specifically used the S-matrix bootstrap to examine string theory and tried to determine whether it is the only consistent quantum gravity theory. "Einstein's theory of General Relativity (GR) describes the gravitational interaction at long distances or (equivalently) low energy," Penedones said. "For example, it can be used to compute how two gravitons of large wavelength (much larger than the Planck length) scatter from each other. However, if we decrease the wavelength at some point, we cannot trust the prediction of GR. In fact, GR's prediction will give probabilities greater than 1."

To improve the reliability of GR's predictions, the theory must be corrected at short distances/wavelength or, equivalently, at high energy. This correction is typically referred to as an 'ultraviolet (UV) completion'. "We often say that a theory of quantum gravity is a UV completion of GR,". "In their recent pape, Guerrieri, Penedones and Pedro Vieira they investigated the first correction to the GR predictions in the low energy limit.

String theory is a renowned theory of quantum gravity. Notably, in string theory, the alpha parameter described by the researchers can take on a specific set of values. In string theory, alpha is related to the tension of the fundamental string (in Planck units), . They set out to explore in this paper was to be agnostic about what is the

theory of quantum gravity which describes the real world and simply ask what values of alpha any such theory could produce."

Surprisingly, the researchers found that the alpha values that a theory of gravity describing the real world could have, according to S-matrix bootstrap numerical calculations, were the exact same values produced by string theory. While these findings could have interesting implications, their study had a couple of limitations that may affect its validity.

So far, they have found that the values of alpha allowed by general principles coincide with those realized in string theory, This is compatible with a positive answer to the question above but it is weak evidence. However, in principle, we can study other parameters, let's call them beta, gamma, etc., representing further sub-leading corrections to the predictions of GR at low energies. There is an infinity of them that String Theory predicts. If we can show that the allowed range of these parameters from the S-matrix Bootstrap principles also coincides with String Theory, then the evidence will be strong."

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